Enric Canadell

List of Publications by Year in Descending Order

425 papers	9,506 citations	50 h-index	71 g-index
496 ext. papers	10,147 ext. citations	6.1 avg, IF	5.82 L-index

#	Paper	IF	Citations
425	Momentum-dependent electron-phonon coupling in charge density wave systems. *Physical Review B*, **2021**, 103,	3.3	2
424	New Radical Cation Salts Based on BDH-TTP Donor: Two Stable Molecular Metals with a Magnetic [ReF6]2−Anion and a Semiconductor with a [ReO4]−Anion. *Magnetochemistry*, **2021**, 7, 54	3.1	1
423	Rich Polymorphism of Layered NbS3. *Chemistry of Materials*, **2021**, 33, 5449-5463	9.6	6
422	Conducting chiral nickel(II) bis(dithiolene) complexes: structural and electron transport modulation with the charge and the number of stereogenic centres. *Journal of Materials Chemistry C*, **2021**, 9, 4119-4140	7.1	6
421	Mixed-valence gold bis(diselenolene) complex turning metallic under pressure. *Journal of Materials Chemistry C*, **2021**, 9, 12291-12302	7.1	3
420	Unusual stoichiometry, band structure and band filling in conducting enantiopure radical cation salts of TM-BEDT-TTF showing helical packing of the donors. *Journal of Materials Chemistry C*, **2021**, 9, 10777-10786	7.1	5
419	Chiral Conducting Me-EDT-TTF and Et-EDT-TTF-Based Radical Cation Salts with the Perchlorate Anion. *Crystals*, **2020**, 10, 1069	2.3	6
418	Weak localization competes with the quantum oscillations in a natural electronic superlattice: The case of Na1.5(PO2)4(WO3)20. *Physical Review B*, **2020**, 101,	3.3	1
417	Nanoscale rotational dynamics of four independent rotators confined in crowded crystalline layers. *Nanoscale*, **2020**, 12, 8294-8302	7.7	7
416	Bilayer Molecular Metal with a Polymeric Anion, β″-(CNB-EDT-TTF)6 Ag~7.95I~9.19. *Crystal Growth and Design*, **2020**, 20, 4224-4227	3.5	3
415	Combining Chirality and Hydrogen Bonding in Methylated Ethylenedithio-Tetrathiafulvalene Primary Diamide Precursors and Radical Cation Salts. *Crystal Growth and Design*, **2020**, 20, 2516-2526	3.5	9
414	Doping of III–V Arsenide and Phosphide Wurtzite Semiconductors. *Journal of Physical Chemistry C*, **2020**, 124, 27203-27212	3.8	1
413	Fermi surface electron-hole instability of the (TMTSF)PF Bechgaard salt revealed by the first-principles Lindhard response function. *Journal of Physics Condensed Matter*, **2020**, 32, 345701	1.8	1
412	Anion ordering transition and Fermi surface electron-hole instabilities in the (TMTSF)ClO and (TMTSF)NO Bechgaard salts analyzed through the first-principles Lindhard response function. *Journal of Physics Condensed Matter*, **2020**, 33, 085705	1.8	0
411	Strain control of the competition between metallic and semiconducting states in single-layers of TaSe3. *2D Materials*, **2020**, 7, 025038	5.9	5
410	Ab initio studies of the optoelectronic structure of undoped and doped silicon nanocrystals and nanowires: the role of size, passivation, symmetry and phase. *Faraday Discussions*, **2020**, 222, 217-239	3.6	4
409	Intermolecular Resonance Correlates Electron Pairs Down a Supermolecular Chain: Antiferromagnetism in K-Doped -Terphenyl. *Journal of the American Chemical Society*, **2020**, 142, 20624-20630	16.4	3

408	In Search of Chiral Molecular Superconductors: [(S,S)-DM-BEDT-TTF] ClO Revisited. *Advanced Materials*, **2020**, 32, e2002811	24	10
407	New insights into the structural properties of (BEDT-TTF)Ag(CN) spin liquid. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2020**, 76, 581-590	1.8	1
406	Conservation of structural arrangements and 3 : 1 stoichiometry in a series of crystalline conductors of TMTTF, TMTSF, BEDT-TTF, and chiral DM-EDT-TTF with the oxo-bis[pentafluorotantalate(v)] dianion. *Chemical Science*, **2020**, 11, 10078-10091	9.4	14
405	Glycine Residue Twists HOMO–HOMO Interactions in a Molecular Conductor. *Crystal Growth and Design*, **2020**, 20, 3546-3554	3.5	1
404	Coexistence of Elastic Modulations in the Charge Density Wave State of 2 H-NbSe. *Nano Letters*, **2019**, 19, 3027-3032	11.5	8
403	Charge Delocalization, Oxidation States, and Silver Mobility in the Mixed Silver-Copper Oxide AgCuO . *Inorganic Chemistry*, **2019**, 58, 7026-7035	5.1	4
402	Fermi surface properties of the bifunctional organic metal (BETS)2Mn[N(CN)2]3 near the metal-insulator transition. *Physical Review B*, **2019**, 99,	3.3	1
401	Electronic structure of the (BEDT-TTF)2I3 surface by photoelectron spectroscopy. *European Physical Journal B*, **2019**, 92, 1	1.2	
400	Polarization dependence of angle-resolved photoemission with submicron spatial resolution reveals emerging one-dimensionality of electrons in NbSe3. *Physical Review B*, **2019**, 99,	3.3	6
399	2D Molecular Superconductor to Insulator Transition in the -(BEDT-TTF)[(HO)(NH)M(CO)]8-crown-6 Series (M = Rh, Cr, Ru, Ir). *Inorganic Chemistry*, **2019**, 58, 10656-10664	5.1	8
398	Magnetic Molecular Conductors Based on Bis(ethylenedithio)tetrathiafulvalene (BEDT-TTF) and the Tris(chlorocyananilato)ferrate(III) Complex. *Inorganic Chemistry*, **2019**, 58, 15359-15370	5.1	7
397	Evidence for the weak coupling scenario of the Peierls transition in the blue bronze. *Physical Review Materials*, **2019**, 3,	3.2	11
396	Electronic engineering of a tetrathiafulvalene charge-transfer salt via reduced symmetry induced by combined substituents. *Physical Chemistry Chemical Physics*, **2019**, 21, 22639-22646	3.6	6
395	Chiral EDT-TTF precursors with one stereogenic centre: substituent size modulation of the conducting properties in the (R-EDT-TTF)2PF6 (R = Me or Et) series. *Journal of Materials Chemistry C* , **2019**, 7, 12664-12673	7.1	13
394	2 2 charge density wave in single-layer TiTe 2. *2D Materials*, **2019**, 6, 015027	5.9	10
393	Preferential Positioning, Stability, and Segregation of Dopants in Hexagonal Si Nanowires. *Nano Letters*, **2019**, 19, 866-876	11.5	9
392	First principles analysis of the CDW instability of single-layer 1 T -TiSe 2 and its evolution with charge carrier density. *2D Materials*, **2018**, 5, 025024	5.9	14
391	Asymmetric Choreography in Pairs of Orthogonal Rotors. *ACS Omega*, **2018**, 3, 1293-1297	3.9	11

390	(CNB-EDT-TTF)4BF4; Anion Disorder Effects in Bilayer Molecular Metals. *Crystals*, **2018**, 8, 142	2.3	7
389	Static Modulation Wave of Arrays of Halogen Interactions Transduced to a Hierarchy of Nanoscale Change Stimuli of Crystalline Rotors Dynamics. *Nano Letters*, **2018**, 18, 3780-3784	11.5	12
388	Stable Metallic State of a Neutral-Radical Single-Component Conductor at Ambient Pressure. *Journal of the American Chemical Society*, **2018**, 140, 6998-7004	16.4	35
387	Strain Tuning of the Anisotropy in the Optoelectronic Properties of TiS3. *ACS Photonics*, **2018**, 5, 3231-3237	6.3	11
386	Donor–anion interactions in quarter-filled low-dimensional organic conductors. *Materials Horizons*, **2018**, 5, 590-640	14.4	33
385	Optical and electronic properties of 2H-MoS2 under pressure: Revealing the spin-polarized nature of bulk electronic bands. *Physical Review Materials*, **2018**, 2,	3.2	14
384	Understanding the Polymerization Process of Eumelanin by Computer Simulations. *Journal of Physical Chemistry C*, **2018**, 122, 28368-28374	3.8	8
383	Conducting Anilate-Based Mixed-Valence Fe(II)Fe(III) Coordination Polymer: Small-Polaron Hopping Model for Oxalate-Type Fe(II)Fe(III) 2D Networks. *Journal of the American Chemical Society*, **2018**, 140, 12611-12621	16.4	40
382	(BEDT-TTF)2Cu2(CN)3 Spin Liquid: Beyond the Average Structure. *Crystals*, **2018**, 8, 158	2.3	13
381	Assessing the Performance of Eumelanin/Si Interface for Photovoltaic Applications. *Journal of Physical Chemistry C*, **2017**, 121, 11576-11584	3.8	11
380	Anisotropic features in the electronic structure of the two-dimensional transition metal trichalcogenide TiS 3 : electron doping and plasmons. *2D Materials*, **2017**, 4, 025085	5.9	20
379	New radical cation salt -(BETS) 2 Co 0.13 Mn 0.87 [N(CN) 2] 3 with two magnetic metals: Synthesis, structure, conductivity and magnetic peculiarities. *Synthetic Metals*, **2017**, 227, 52-60	3.6	4
378	Quantum oscillations in coupled orbits networks of (BEDT-TTF) salts with tris(oxalato)metallate anions. *Low Temperature Physics*, **2017**, 43, 27-33	0.7	2
377	Synthesis and Physical Properties of Purely Organic BEDT-TTF-Based Conductors Containing Hetero-/Homosubstituted Cl/CN-Anilate Derivatives. *Inorganic Chemistry*, **2017**, 56, 12564-12571	5.1	12
376	Electronic structure of 2 H -NbSe 2 single-layers in the CDW state. *2D Materials*, **2016**, 3, 035028	5.9	33
375	Polymorphism and Superconductivity in Bilayer Molecular Metals (CNB-EDT-TTF)I. *Inorganic Chemistry*, **2016**, 55, 10343-10350	5.1	13
374	Single-Component Conductors: A Sturdy Electronic Structure Generated by Bulky Substituents. *Inorganic Chemistry*, **2016**, 55, 6036-46	5.1	18
373	Charge transfer and 2k F vs. 4k F instabilities in the NMP-TCNQ molecular metal and (NMP) x (Phen) 1- TCNQ solid solutions. *Europhysics Letters*, **2016**, 113, 27006	1.6	8

372	Correlating conduction properties with the molecular symmetry: segregation of Z and E isomers in the charge-assisted, halogen-bonded cocrystal [(Z,E)-Me2I2TTF]2Br. *Chemical Communications*, **2016**, 52, 308-11	5.8	6
371	Nanotexturing To Enhance Photoluminescent Response of Atomically Thin Indium Selenide with Highly Tunable Band Gap. *Nano Letters*, **2016**, 16, 3221-9	11.5	119
370	Localization versus Delocalization in Chiral Single Component Conductors of Gold Bis(dithiolene) Complexes. *Journal of the American Chemical Society*, **2016**, 138, 6838-51	16.4	37
369	Anion size control of the packing in the metallic versus semiconducting chiral radical cation salts (DM-EDT-TTF)XF (X = P, As, Sb). *Chemical Communications*, **2016**, 52, 12438-12441	5.8	27
368	Near-Edge X-ray Absorption Fine Structure Investigation of the Quasi-One-Dimensional Organic Conductor (TMTSF)PF. *Journal of Physical Chemistry A*, **2016**, 120, 8574-8583	2.8	2
367	Nature of the empty states and signature of the charge density wave instability and upper Peierls transition of TTF-TCNQ by temperature-dependent NEXAFS spectroscopy. *European Physical Journal B*, **2015**, 88, 1	1.2	10
366	Exploring the electronic structure of an organic semiconductor based on a compactly fused electron donor-acceptor molecule. *ChemPhysChem*, **2015**, 16, 1361-5	3.2	6
365	Bilayer Molecular Metals Based on Dissymmetrical Electron Donors. *Inorganic Chemistry*, **2015**, 54, 6677-9	5.1	15
364	Donor-anion interactions at the charge localization and charge ordering transitions of (TMTTF)2AsF6 probed by NEXAFS. *Physical Chemistry Chemical Physics*, **2015**, 17, 19202-14	3.6	12
363	Metal-charge density wave coexistence in TTF[Ni(dmit)2]2. *Physica B: Condensed Matter*, **2015**, 460, 147-150	1.8	
362	Complete series of chiral paramagnetic molecular conductors based on tetramethyl-bis(ethylenedithio)-tetrathiafulvalene (TM-BEDT-TTF) and Chloranilate-bridged heterobimetallic honeycomb layers. *Inorganic Chemistry*, **2015**, 54, 3643-53	5.1	50
361	Gearing motion in cogwheel pairs of molecular rotors: weak-coupling limit. *CrystEngComm*, **2015**, 17, 7829-7834	3.3	20
360	Links between the Crystal and Electronic Structure in the New Family of Unconventional Superconductors A2Cr3As3 (A = K, Rb, Cs). *Inorganic Chemistry*, **2015**, 54, 8029-34	5.1	15
359	Non-Lifshitz-Kosevich field- and temperature-dependent amplitude of quantum oscillations in the quasi-two dimensional metal κ-(ET)2InBr(C2H4Cl2). *Journal of Physics Condensed Matter*, **2015**, 27, 315601	1.8	3
358	Quasiparticle spectra of 2H-NbSe2: Two-band superconductivity and the role of tunneling selectivity. *Physical Review B*, **2015**, 92,	3.3	32
357	Tunneling and electronic structure of the two-gap superconductor MgB2. *Physical Review B*, **2015**, 92,	3.3	5
356	Effect of Halopyridine Guest Molecules on the Structure and Superconducting Properties of β-[Bis(ethylenedithio)tetrathiafulvalene]4(H3O)[Fe(C2O4)3]·Guest Crystals. *European Journal of Inorganic Chemistry*, **2015**, 2015, 5611-5620	2.3	14
355	Structural and electronic control of the metal to insulator transition and local orderings in the κ-(BEDT-TTF)2X organic conductors. *Journal of Physics Condensed Matter*, **2015**, 27, 465702	1.8	12

354	Enantiopure Conducting Salts of Dimethylbis(ethylenedithio)tetrathiafulvalene (DM-BEDT-TTF) with the Hexachlororhenate(IV) Anion. *European Journal of Inorganic Chemistry*, **2014**, 2014, 3855-3862	2.3	28
353	Electrical magnetochiral anisotropy in a bulk chiral molecular conductor. *Nature Communications*, **2014**, 5, 3757	17.4	132
352	Charge density wave and metallic state coexistence in the multiband conductor TTF[Ni(dmit)2]2. *Physical Review B*, **2014**, 90,	3.3	10
351	Electronic structure, optical properties, and lattice dynamics in atomically thin indium selenide flakes. *Nano Research*, **2014**, 7, 1556-1568	10	132
350	Changing gears to neutral in a polymorph of one-dimensional arrays of cogwheel-like pairs of molecular rotors. *CrystEngComm*, **2014**, 16, 1241	3.3	14
349	Nature of holes, oxidation states, and hypervalency in covellite (CuS). *Inorganic Chemistry*, **2014**, 53, 12402-6	5.1	49
348	On a new FeOF polymorph: Synthesis and stability. *Solid State Sciences*, **2014**, 38, 55-61	3.4	4
347	Dual-Layered Quasi-Two-Dimensional Organic Conductors with Presumable Incoherent Electron Transport. *European Journal of Inorganic Chemistry*, **2014**, 2014, 3820-3836	2.3	16
346	Reversible Control of Crystalline Rotors by Squeezing Their Hydrogen Bond Cloud Across a Halogen Bond-Mediated Phase Transition. *Crystal Growth and Design*, **2014**, 14, 3375-3383	3.5	30
345	C□□BF2O2 Interactions in Crystals: A Case for Boron Hydrogen Bonding?. *Crystal Growth and Design*, **2014**, 14, 3700-3703	3.5	8
344	De Haas-van Alphen oscillations in the compensated organic metal □pseudo-□-(ET)4H3O[Fe(C2O4)3]□(C6H4Br2). *European Physical Journal B*, **2014**, 87, 1	1.2	2
343	Structural diversity and physical properties of paramagnetic molecular conductors based on bis(ethylenedithio)tetrathiafulvalene (BEDT-TTF) and the tris(chloranilato)ferrate(III) complex. *Inorganic Chemistry*, **2014**, 53, 7028-39	5.1	36
342	Electronic structure and anion ordering in (TMTSF)2ClO4 and (TMTSF)2NO3: A first-principles study. *Physical Review B*, **2014**, 89,	3.3	25
341	Chemical Bonding in Solids **2014**, 445-476		
340	A Crystalline Hybrid of Paddlewheel Copper(II) Dimers and Molecular Rotors: Singlet-triplet Dynamics Revealed by Variable-temperature Proton Spin-lattice Relaxation. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2014**, 640, 1127-1133	1.3	13
339	Fermi surface and effect of high magnetic fields on the metal-semimetal Peierls-like transition of (TSeT)2Cl. *Low Temperature Physics*, **2014**, 40, 307-310	0.7	
338	The first molecular superconductor based on BEDT-TTF radical cation salt with paramagnetic tris(oxalato)ruthenate anion. *CrystEngComm*, **2013**, 15, 7048	3.3	25
337	Electronic Conductivity of Solids **2013**, 1007-1034		

336	Correlation between Metal□Insulator Transition and Hydrogen-Bonding Network in the Organic Metal □(BEDT-TTF)4[2,6-Anthracene-bis(sulfonate)]□(H2O)4. *Crystal Growth and Design*, **2013**, 13, 5135-5145	3.5	7
335	Chirality driven metallic versus semiconducting behavior in a complete series of radical cation salts based on dimethyl-ethylenedithio-tetrathiafulvalene (DM-EDT-TTF). *Journal of the American Chemical Society*, **2013**, 135, 17176-86	16.4	70
334	Factors affecting the magnetic coupling in Sr2V3O9 type oxides: As for V substitution in the VO4 tetrahedra and nature of the cation. *Dalton Transactions*, **2013**, 42, 15555-8	4.3	
333	Onsager phase factor of quantum oscillations in the organic metal □(BEDT-TTF)4CoBr4(C6H4Cl2). *Synthetic Metals*, **2013**, 171, 51-55	3.6	8
332	Robust Dirac-cone band structure in the molecular kagome compound (EDT-TTF-CONH2)6[Re6Se8(CN)6]. *Inorganic Chemistry*, **2013**, 52, 3326-33	5.1	7
331	Crystalline arrays of pairs of molecular rotors: correlated motion, rotational barriers, and space-inversion symmetry breaking due to conformational mutations. *Journal of the American Chemical Society*, **2013**, 135, 9366-76	16.4	81
330	Structural phase transition in the □?-(BEDT-TTF)4H3O[Fe(C2O4)3]□G crystals (where G is a guest solvent molecule). *CrystEngComm*, **2012**, 14, 460-465	3.3	18
329	Anisotropic chemical pressure effects in single-component molecular metals based on radical dithiolene and diselenolene gold complexes. *Journal of the American Chemical Society*, **2012**, 134, 17138-48	16.4	65
328	NH3 molecular doping of silicon nanowires grown along the [112], [110], [001], and [111] orientations. *Nanoscale Research Letters*, **2012**, 7, 308	5	20
327	Role of p-d and s-d interactions in the electronic structure and band gap of Zn1□MxO (M=Cr, Mn, Fe, Co, Ni, and Cu): Photoelectron and optical spectroscopy and first-principles band structure calculations. *Physical Review B*, **2012**, 86,	3.3	37
326	Quantum oscillations in the linear chain of coupled orbits: The organic metal with two cation layers □(ET) 4 CoBr 4 (C 6 H 4 Cl 2). *Europhysics Letters*, **2012**, 97, 57003	1.6	22
325	Design and evaluation of a crystalline hybrid of molecular conductors and molecular rotors. *Journal of the American Chemical Society*, **2012**, 134, 7880-91	16.4	48
324	Single-Crystal-to-Single-Crystal Transformation from □(BEDT-TTF)4[OsNOCl5]1.33(C6H5NO2)0.67 to □-(BEDT-TTF)3[OsNOCl5]. *Crystals*, **2012**, 2, 627-642	2.3	1
323	Charge ordering in low dimensional organic conductors: Structural aspects. *Physica Status Solidi (B): Basic Research*, **2012**, 249, 937-942	1.3	20
322	Essential role of anions in the charge ordering transition of □(BEDT-TTF)2I3. *Physical Review B*, **2012**, 85,	3.3	62
321	Orbital Approach to the Electronic Structure of Solids **2012**,		19
320	Dual [proton]/[hole] mixed valence in a molecular metal: balancing chemical activity in the solid state by tapping into a molecular hole reservoir. *Journal of Materials Chemistry*, **2011**, 21, 1516-1522		11
319	□pseudo-□(BEDT-TTF)4(H3O)[Fe(C2O4)3]□C6H4Br2. *CrystEngComm*, **2011**, 13, 2430	3.3	27

318	Electronic structure of the two-leg spin ladder (C5H12N)2CuBr4. *Inorganic Chemistry*, **2011**, 50, 6399-401	5.1	2
317	Syntheses, crystal structures, transport properties and first-principles electronic structure study of the (tTTF)2X (X=Br, I) low-dimensional antiferromagnets. *Inorganic Chemistry*, **2011**, 50, 4171-81	5.1	9
316	The metallic transport of (TMTSF)2X organic conductors close to the superconducting phase. *Journal of Physics Condensed Matter*, **2011**, 23, 345702	1.8	10
315	Temperature- and pressure-dependent metallic states in (BEDT□TTF)8[Hg4Br12(C6H5Br)2]. *Physical Review B*, **2011**, 84,	3.3	5
314	Magnetoresistance oscillations up to 32 K in the organic metal □-(ET)4(H3O)[Fe(C2O4)3] □C6H4Cl2. *Low Temperature Physics*, **2011**, 37, 749-754	0.7	3
313	An efficient computational method for use in structural studies of crystals with substitutional disorder. *Journal of Physics Condensed Matter*, **2010**, 22, 415401	1.8	6
312	Quantum interference and Shubnikov□de Haas oscillations in □-(ET)4(H3O)[Fe(C2O4)3]□C6H4Cl2 under pressure. *Synthetic Metals*, **2010**, 160, 2467-2470	3.6	3
311	First-principles study of the interaction between paramagnetic V4+ centers through formally magnetically inactive VO4 tetrahedra in the quasi-one-dimensional spin systems Sr2V3O9 and Ba2V3O9. *Physical Review B*, **2010**, 82,	3.3	4
310	Density-wave instability in □BEDT-TTF)2KHg(SCN)4 studied by x-ray diffuse scattering and by first-principles calculations. *Physical Review B*, **2010**, 82,	3.3	22
309	Temperature-pressure phase diagram and electronic properties of the organic metal □BETS)2Mn[N(CN)2]3. *Physical Review B*, **2010**, 82,	3.3	16
308	Order versus disorder in chiral tetrathiafulvalene-oxazoline radical-cation salts: structural and theoretical investigations and physical properties. *Chemistry - A European Journal*, **2010**, 16, 528-37	4.8	44
307	A neutral zwitterionic molecular solid. *Chemistry - A European Journal*, **2010**, 16, 14051-9	4.8	35
306	Magnetotransport properties of a new hybrid metal □(BEDT-TTF)2[Mn2Cl5(H2O)5]. *Physica B: Condensed Matter*, **2010**, 405, S247-S249	2.8	1
305	The first polymorph, □-(ET)2Cu[N(CN)2]Cl, in the family of □(ET)2Cu[N(CN)2]X (X=Cl, Br, I) radical cation salts. *Journal of Solid State Chemistry*, **2009**, 182, 617-621	3.3	8
304	Uniform linear chains of group 11 atoms: do they have a bias towards a Peierls distortion?. *Theoretical Chemistry Accounts*, **2009**, 123, 85-92	1.9	3
303	Indications for the coexistence of closed orbit and quantum interferometer with the same cross section in the organic metal □?-(ET)4(H3O)[Fe(C2O4)3] .C6H4Cl2: persistence of Shubnikov-de Haas oscillations above 30 K. *European Physical Journal B*, **2009**, 71, 203-209	1.2	5
302	Electronic structure and spin exchange interactions in Na(2)V(3)O(7): a vanadium(IV) oxide nanotubular phase. *Inorganic Chemistry*, **2009**, 48, 5779-89	5.1	6
301	Electronic structure of the A(8)Tr(11) (A = K, Rb, Cs; Tr = Ga, In, Tl) Zintl phases: possible chemical reasons behind their activated versus non activated conductivity. *Inorganic Chemistry*, **2009**, 48, 9792-9	5.1	4

300	Host-guest interactions, uniform vs fragmented linear atom chains and likeliness of Peierls distortions in the (Ca7N4)[M(x)] (M = Ag, Ga, In) phases. *Inorganic Chemistry*, **2009**, 48, 2919-31	5.1	2
299	Concerning the possibility of hidden one-dimensional Fermi surfaces for the K(0.25)WO(3) hexagonal bronze. *Inorganic Chemistry*, **2009**, 48, 11492-4	5.1	2
298	A new hybrid molecular metal assembling a BEDT-TTF conducting network and the magnetic chain anion [Mn2Cl5(H2O)5]□□(BEDT-TTF)2[Mn2Cl5(H2O)5]. *CrystEngComm*, **2009**, 11, 2102	3.3	4
297	A single-component molecular metal based on a thiazole dithiolate gold complex. *Journal of the American Chemical Society*, **2009**, 131, 16961-7	16.4	92
296	Chemical effects on the optical band-gap of heavily doped ZnO:MIII (M=Al,Ga,In): An investigation by means of photoelectron spectroscopy, optical measurements under pressure, and band structure calculations. *Physical Review B*, **2009**, 79,	3.3	106
295	CaFeO2: a new type of layered structure with iron in a distorted square planar coordination. *Journal of the American Chemical Society*, **2009**, 131, 221-9	16.4	80
294	Molecular conductors based on the mixed-valence polyoxometalates [SMo12O40]n- (n = 3 and 4) and the organic donors bis(ethylenedithio)tetrathiafulvalene and bis(ethylenedithio)tetraselenafulvalene. *Inorganic Chemistry*, **2009**, 48, 11314-24	5.1	19
293	Charge ordering, symmetry and electronic structure issues and Wigner crystal structure of the quarter-filled band Mott insulators and high pressure metals □(EDT-TTF-CONMe2)2X, X = Br and AsF6. *Journal of Materials Chemistry*, **2009**, 19, 6980		44
292	Marcasite vs.arsenopyrite structural choice in MN2 (M = Ir, Os and Rh) transition metal nitrides. *Journal of Materials Chemistry*, **2008**, 18, 2090		19
291	The 8 : 1 : 1 ternary hybrid framework in the system [EDT-TTF +][1,4-bis(iodoethynyl)benzene][Re6Se8(CN)6]4-: dual noncovalent expression of the octahedral halogen-bond hexa-acceptor nanonode. *Chemical Communications*, **2008**, 2194-6	5.8	33
290	Magnetic oscillations amplitude of a dirty quasi two-dimensional organic metal. *Synthetic Metals*, **2008**, 158, 973-976	3.6	2
289	Conducting mixed-valence salt of bis(ethylenedithio)tetrathiafulvalene (BEDT-TTF) with the paramagnetic heteroleptic anion [CrIII(oxalate)2(2,2?-bipyridine)]□*New Journal of Chemistry*, **2008**, 32, 333-339	3.6	19
288	The family of molecular conductors [(n-Bu)4N]2[M(dcbdt)2]5, M = Cu, Ni, Au; band filling and stacking modulation effects. *Journal of Materials Chemistry*, **2008**, 18, 2825		18
287	Modulating the framework negative charge density in the system [BDT-TTP*+]/[Re6S5Cl9(1-)]/[Re6(S/Se)6Cl8(2-)]/[Re6S7Cl7(3-)]: templating by isosteric cluster anions of identical symmetry and shape, variations of incommensurate band filling, and electronic structure in 2D metals. *Journal of the American Chemical Society*, **2008**, 130, 3235-48	16.4	23
286	Structural and electronic properties of SrFeO2 from first principles. *Physical Review B*, **2008**, 78,	3.3	63
285	High-pressure electronic structure and phase transitions in monoclinic InSe: X-ray diffraction, Raman spectroscopy, and density functional theory. *Physical Review B*, **2008**, 77,	3.3	31
284	Roles of cations, electronegativity difference, and anionic interlayer interactions in the metallic versus nonmetallic character of Zintl phases related to arsenic. *Journal of Computational Chemistry*, **2008**, 29, 2144-53	3.5	24
283	Shubnikov-de Haas oscillations spectrum of the strongly correlated quasi-2D organic metal (ET)8[Hg4Cl12(C6H5Br)2] under pressure. *European Physical Journal B*, **2008**, 66, 489-495	1.2	8

282	Structural phase transition in crystals of the molecular conductor 2-(BDH-TTP)6[Hg(SCN)3][Hg(SCN)4]. *Crystallography Reports*, **2008**, 53, 1003-1008	0.6	1
281	The staging influence on the electronic structure and transport of superconducting sodium-doped hafnium nitride chloride. *Journal of Materials Chemistry*, **2007**, 17, 4362		2
280	O?S vs. N?S intramolecular nonbonded interactions in neutral and radical cation salts of TTF-oxazoline derivatives: synthesis, theoretical investigations, crystalline structures, and physical properties. *New Journal of Chemistry*, **2007**, 31, 1468	3.6	56
279	Intramolecular mixed-valence state through silicon or germanium double bridges in rigid bis(tetrathiafulvalenes). *Chemistry - A European Journal*, **2007**, 13, 5394-400	4.8	31
278	Transport measurements under pressure in III-IV layered semiconductors. *Physica Status Solidi (B): Basic Research*, **2007**, 244, 162-168	1.3	10
277	GaS and InSe equations of state from single crystal diffraction. *Physica Status Solidi (B): Basic Research*, **2007**, 244, 169-173	1.3	7
276	Crystal structure, Fermi surface calculations and Shubnikov-de Haas oscillation spectrum of the organic metal (BETS)4HgBr4(C6H5Cl) at low temperature. *Solid State Sciences*, **2007**, 9, 1140-1148	3.4	16
275	Frequency combinations in the magnetoresistance oscillations spectrum of a linear chain of coupled orbits with a high scattering rate. *European Physical Journal B*, **2007**, 55, 383-388	1.2	7
274	First radical cation salts of 2,5-bis(1,3-dithian-2-ylidene)-1,3,4,6-tetrathiapentalene (BDA-TTP) with copper(II) metal complex anions: (BDA-TTP)4Cu2Cl6 and (BDA-TTP)2CuCl4. *Russian Chemical Bulletin*, **2007**, 56, 49-55	1.7	
273	Monoclinic Polymorphs of the Bechgaard-Fabre Salts. *Journal of Low Temperature Physics*, **2007**, 142, 401-404	1.3	
272	First-principles study of the electronic structure of cubic GaS: Metallic versus insulating polymorphs. *Physical Review B*, **2007**, 75,	3.3	4
271	Inhomogenities of the CDW vector at the (-201) surface of Quasi-1D blue bronze Rb0.3MoO3. *Journal of Physics: Conference Series*, **2007**, 61, 140-146	0.3	2
270	New BEDT-TTF/[Fe(C5O5)3]3- hybrid system: synthesis, crystal structure, and physical properties of a chirality-induced alpha phase and a novel magnetic molecular metal. *Inorganic Chemistry*, **2007**, 46, 4446-57	5.1	30
269	Monoclinic polymorphs of the bechgaard-fabre salts. *Journal of Low Temperature Physics*, **2006**, 142, 397-400	1.3	1
268	Pressure dependence of Shubnikov-de Haas oscillation spectra in the quasi-two-dimensional organic metal (BEDT-TTF)4(NH4)[Fe(C2O4)3]·DMF. *Physical Review B*, **2006**, 74,	3.3	6
267	Transport properties and structural features of the ambient-pressure superconductor (BEDT-TTF)2Cu[N(CN)2]Cl. *Physical Review B*, **2006**, 74,	3.3	13
266	High-pressure, high-temperature phase diagram of InSe: A comprehensive study of the electronic and structural properties of the monoclinic phase of InSe under high pressure. *Physical Review B*, **2006**, 73,	3.3	32
265	Electronic Structure of Solids **2006**,		1

264	A chirality-induced alpha phase and a novel molecular magnetic metal in the BEDT-TTF/tris(croconate)ferrate(III) hybrid molecular system. *Chemical Communications*, **2006**, 4931-3	5.8	31
263	Molecular conductors with the common and robust building block (BEDT-TTF)2NP (NP = [FeNO(CN)5]2−) but different band filling. *Journal of Materials Chemistry*, **2006**, 16, 787		2
262	Analysis of scanning tunneling microscopy images of the charge-density-wave phase in quasi-one-dimensional Rb0.3MoO3. *Physical Review B*, **2006**, 74,	3.3	6
261	Electronic structure and charge transfer in the ternary intercalated graphite beta-KS0.25C3. *Inorganic Chemistry*, **2006**, 45, 9387-93	5.1	
260	Nature of the bottom t2g-block bands of layered perovskites. Implications for the transport properties of phases where these bands are partially filled. *Journal of the American Chemical Society*, **2006**, 128, 4318-29	16.4	11
259	Concerning the different roles of cations in metallic Zintl phases: Ba7Ga4Sb9 as a test case. *Inorganic Chemistry*, **2006**, 45, 7235-41	5.1	20
258	Pressure dependence of the Shubnikov-de Haas oscillation spectrum of (beta'')-(BEDT-TTF)4(NH4)[Cr(C2 O4)3] .DMF. *European Physical Journal B*, **2006**, 51, 53-60	1.2	11
257	Multistability in a family of DTTTF organic radical based compounds (DTTTF)4[M(L)2]3 (M = Au, Cu; L = pds, pdt, bdt). *Journal of Materials Chemistry*, **2005**, 15, 3187		26
256	New molecular metals based on BEDO radical cation salts with the square planar Ni(CN)42− anion. *Journal of Materials Chemistry*, **2005**,		1
255	Concerning the Structure of Hydrogen Molybdenum Bronze Phase III. A Combined Theoretical−Experimental Study. *Chemistry of Materials*, **2005**, 17, 5957-5969	9.6	41
254	Electronic structure of Li2Ga and Li9Al4, two solids containing infinite and uniform zigzag chains. *Inorganic Chemistry*, **2005**, 44, 374-81	5.1	5
253	Electronic structure of the K3Bi2 metallic phase. *Inorganic Chemistry*, **2005**, 44, 1644-6	5.1	7
252	Crystalline patterns and band structure dimensionality in a series of conducting hybrids associating amide-functionalized EDT-TTF donors with the isosteric octahedral anions [FeNO(CN)5]2− and [M(CN)6]3− (M = Co, Fe). *Synthetic Metals*, **2005**, 155, 527-538	3.6	4
251	The first BDH-TTP radical cation salts with mercuric counterions, (BDH-TTP)4[Hg(SCN)4]·C6H5NO2 and (BDH-TTP)6[Hg(SCN)3][Hg(SCN)4]. *Synthetic Metals*, **2005**, 155, 588-594	3.6	10
250	Crystal symmetry and pressure effects on the valence band structure of InSe and GaSe: Transport measurements and electronic structure calculations. *Physical Review B*, **2005**, 71,	3.3	54
249	Chiral molecular metals: syntheses, structures, and properties of the AsF(6)(-) salts of racemic (+/-)-, (R)-, and (S)-tetrathiafulvalene-oxazoline derivatives. *Journal of the American Chemical Society*, **2005** , 127, 5748-9	16.4	86
248	Variety of molecular conducting layers in the family of radical cation salts based on BEDT-TTF with the metal mononitrosyl complex [OsNOCl5]2− *Journal of Materials Chemistry*, **2005**, 15, 2476		14
247	(EDT-TTF-CONH2)6[Re6Se8(CN)6], a metallic Kagome-type organic-inorganic hybrid compound: electronic instability, molecular motion, and charge localization. *Journal of the American Chemical Society*, **2005**, 127, 11785-97	16.4	78

246	Monoclinic Polymorphs of Bechgaard and Fabre Salts. *Advanced Materials*, **2005**, 17, 209-212	24	9
245	Exploitation of the photochromic nitroprusside anion [FeNO(CN)5]2-as counterion for constructing molecular conductors: The first radical cation salts based on BDH-TTP and the amide functionalized derivatives of EDT-TTF. *European Physical Journal Special Topics*, **2004**, 114, 481-485		6
244	Band structure of indium selenide investigated by intrinsic photoluminescence under high pressure. *Physical Review B*, **2004**, 70,	3.3	28
243	Combination frequencies of magnetic oscillations in □(BEDT□TTF)4(NH4)[Fe(C2O4)3]?DMF. *Physical Review B*, **2004**, 69,	3.3	29
242	Electronic band structure of □(Per)2M(mnt)2 compounds. *European Physical Journal B*, **2004**, 42, 453-456	1.2	20
241	Step-by-Step Construction of the Electronic Structure of Molecular Conductors: Conceptual Aspects and Applications. *Advanced Functional Materials*, **2004**, 14, 201-214	15.6	27
240	New Organic Metals Based on BDH-TTP Radical Cation Salts with the Photochromic Nitroprusside Anion [FeNO(CN)5]2□*Advanced Functional Materials*, **2004**, 14, 660-668	15.6	20
239	Electron-Rich Organoantimony(III) Dithiolate Complexes. *European Journal of Inorganic Chemistry*, **2004**, 2004, 3409-3414	2.3	10
238	Synthesis, characterization, and electronic structure of Ba5In4Bi5: an acentric and one-electron deficient phase. *Chemistry - A European Journal*, **2004**, 10, 3615-21	4.8	29
237	Structural isomerism in crystals of redox-active secondary ortho-diamides: the role of competing intra- and intermolecular hydrogen bonds in directing crystalline topologies. *Chemistry - A European Journal*, **2004**, 10, 4498-511	4.8	45
236	Magnetic oscillations in □-(BEDT□TTF)4(NH4)[Fe(C2O4)3]□DMF: Fermi surface study and frequency mixing. *Physica B: Condensed Matter*, **2004**, 346-347, 359-362	2.8	
235	Concerning the origin of superstructures in hydrogen molybdenum bronzes HxMoO3. *Solid State Ionics*, **2004**, 168, 291-298	3.3	6
234	Global instability index optimizations for the localization of mobile protons. *Solid State Ionics*, **2004**, 168, 281-290	3.3	42
233	Synthesis, crystal structure, and physical properties of (BEDT-TTF)[Ni(tdas)2] (BEDT-TTF = bis(ethylenedithio)tetrathiafulvalene; tdas = 1,2,5-thiadiazole-3,4-dithiolate): first monomeric [Ni(tdas)2]- monoanion. *Inorganic Chemistry*, **2004**, 43, 2049-56	5.1	25
232	(EDT-TTF-I2)2PbI3□H2O: an ambient pressure metal with a □ donor slab topology. *Journal of Materials Chemistry*, **2004**, 14, 135-137		32
231	Superstructures of donor packing arrangements in a series of molecular charge transfer salts. *Chemical Communications*, **2004**, 18-9	5.8	44
230	A chiral molecular conductor: synthesis, structure, and physical properties of [ET]3[Sb2(L-tart)2].CH3CN (ET = bis(ethylendithio)tetrathiafulvalene; L-tart = (2R,3R)-(+)-tartrate). *Inorganic Chemistry*, **2004**, 43, 8072-7	5.1	59
229	Antifluorite-type lithium chromium oxide nitrides: synthesis, structure, order, and electrochemical properties. *Inorganic Chemistry*, **2004**, 43, 7050-60	5.1	35

228	Single-component magnetic conductors based on Mo3S7 trinuclear clusters with outer dithiolate ligands. *Journal of the American Chemical Society*, **2004**, 126, 12076-83	16.4	83
227	Comments on the paper Infrared reflectance spectra of the organic conductor (BEDT-TTF)4K[Fe(CN)5NO]2 by R. Swietlik, B. Zhang, Y.X. Yao, H.X. Li, D.B. Zhu, published in Synthetic Metals 129 (2002) 95100.. *Synthetic Metals*, **2004**, 140, 105-106	3.6	
226	New molecular conductors based on EDT with anionic complexes of rare-earth elements: (EDT)2[Ho(NCS)4(H2O)4] and (EDT)3[Y(NO3)5]. *Synthetic Metals*, **2004**, 143, 221-228	3.6	3
225	Computing the Properties of Materials from First Principles with SIESTA. *Structure and Bonding*, **2004**, 103-170	0.9	96
224	Transport, Magnetic and Optical Properties of a Quasi-Two-Dimensional Organic Metal Based on BEDO-TTF (Bis-(Ethylenedioxy) Tetrathiafulvalene) **2004**, 309-318		
223	Molecular Metals Based on BEDT-TTF Radical Cation Salts with Magnetic Metal Oxalates as Counterions: -(BEDT-TTF)4A[M(C2O4)3]DMF (A = NH4+, K+; M = CrIII, FeIII). *Advanced Functional Materials*, **2003**, 13, 403-411	15.6	77
222	A Genuine Quarter-Filled Band Mott Insulator, (EDT-TTF-CONMe2)2AsF6: Where the Chemistry and Physics of Weak Intermolecular Interactions Act in Unison. *Advanced Materials*, **2003**, 15, 1251-1254	24	51
221	Quantitative vs. qualitative approaches to the electronic structure of solids. *Journal of Solid State Chemistry*, **2003**, 176, 375-389	3.3	8
220	Specific features of the electronic structure of III VI layered semiconductors: recent results on structural and optical measurements under pressure and electronic structure calculations. *Physica Status Solidi (B): Basic Research*, **2003**, 235, 267-276	1.3	17
219	Localized versus delocalized bonding in the K5Bi4 metallic salt. *Inorganic Chemistry*, **2003**, 42, 2759-63	5.1	17
218	Singular crystalline beta'-layered topologies directed by ribbons of self-complementary amide...amide ring motifs in [EDT-TTF-(CONH(2))(2)](2)X (X = HSO(4)(-), ClO(4)(-), ReO(4)(-), AsF(6)(-)): coupled activation of ribbon curvature, electron interactions, and magnetic susceptibility. *Journal of the American Chemical Society*, **2003**, 125, 11582-90	16.4	59
217	Single crystalline commensurate metallic assemblages of pi-slabs and CdI2-type layers: synthesis and properties of beta-(EDT-TTF-I2)2[Pb5/6 square 1/6I2](3) and beta-(EDT-TTF-I2)2[Pb2/3+xAg1/3-2x square xI2]3, x = 0.05. *Journal of the American Chemical Society*, **2003**, 125, 2295-301	16.4	85
216	Interdependence of redox state, hydrogen bonding, anion recognition and charge partition in crystals of (EDT-TTF-CONHMe)6 [Re6Se8(CN)6] (CH3CN)2(CH2Cl2)2. *Chemical Communications*, **2003**, 1820-1	5.8	18
215	Crystal and electronic structures of a new metallic modification of the (ET)2[KHg(SCN)4]. *Synthetic Metals*, **2003**, 133-134, 467-468	3.6	1
214	Crystal and electronic structure of new molecular semiconductors (ET)5[M(NCS)6NO3]C2H5OH (M=Dy, Y, Ho) and (TMTSF)3[Y(NO3)5]2C6H5Cl. *Synthetic Metals*, **2003**, 133-134, 389-391	3.6	
213	Structure-properties relationships in organic molecular conductors based on radical cation salts with octahedral metal complexes as counterions. *Synthetic Metals*, **2003**, 133-134, 373-375	3.6	7
212	Characterization of the unoccupied and partially occupied states of TTF-TCNQ by XANES and first-principles calculations. *Physical Review B*, **2003**, 68,	3.3	50
211	First-principles characterization of the electronic structure of the molecular superconductor (BEDTTTF)2IBr2. *Physical Review B*, **2003**, 67,	3.3	17

210	An in-depth correlation of perturbation of the organic-inorganic interface topology, electronic structure, and transport properties within beta''-(BEDT-TTF)(4) x (guest)(n) x [Re(6)Q(6)Cl(8)], (Q=S, Se). *Chemistry - A European Journal*, **2002**, 8, 3884-900	4.8	27
209	Fluorine Segregation Controls the Solid-State Organization and Electronic Properties of Ni and Au Dithiolene Complexes: Stabilization of a Conducting Single-Component Gold Dithiolene Complex. *Advanced Functional Materials*, **2002**, 12, 693-698	15.6	53
208	Rare-Earth Elements in Molecular Conductors: Crystal and Electronic Structures. *Journal of Solid State Chemistry*, **2002**, 168, 457-463	3.3	10
207	The First Mixed Valence Radical Cation Salts of BEDT-TTF with the Photochromic Metal Mononitrosyl Complexes [RuNOX5]2□(X=Br, Cl) as Counterions. *Journal of Solid State Chemistry*, **2002**, 168, 514-523	3.3	13
206	A New Conducting Molecular Solid Based on the Magnetic [Ni(dmf)6]2+ Cation and on [Ni(dsit)2]22□(dsit=1,3-dithiole-2-thione-4,5-diselenolate) Showing an Unprecedented Anion Packing. *Journal of Solid State Chemistry*, **2002**, 168, 653-660	3.3	8
205	Crystal and electronic structures of new molecular semiconductors with trinitroresorcinol anions. *Physica E: Low-Dimensional Systems and Nanostructures*, **2002**, 13, 1268-1270	3	3
204	Quasi-three-dimensional network of molecular interactions and electronic structure of a new organic semiconductor, ET(NCS)0.77. *Acta Crystallographica Section B: Structural Science*, **2002**, 58, 148-52		4
203	Crystal and electronic structure of a new metallic modification of (ET)2[KHg(SCN)4]. *Acta Crystallographica Section B: Structural Science*, **2002**, 58, 471-6		2
202	Electronic localization in an extreme 1-D conductor: the organic salt (TTDM-TTF) [Au(mnt)]. *European Physical Journal B*, **2002**, 29, 27-33	1.2	15
201	First-principles study of the blue bronze K0.3MoO3. *Physical Review B*, **2002**, 65,	3.3	36
200	First-principles study of the neutral molecular metal Ni(tmdt)2. *Physical Review B*, **2002**, 65,	3.3	55
199	New Molecular Conductors Based on ETEDT-TTF Trihalides: From Single Crystals to Conducting Layers of Nanocrystals. *Chemistry of Materials*, **2002**, 14, 3295-3304	9.6	12
198	Angle-resolved photoemission study and first-principles calculation of the electronic structure of GaTe. *Physical Review B*, **2002**, 65,	3.3	34
197	Electronic structure, electrical and magnetic properties of RMo(8)O(14) compounds (R = La, Ce, Pr, Nd, Sm) containing bicapped Mo(8) clusters. *Inorganic Chemistry*, **2002**, 41, 4689-99	5.1	18
196	Interesting transport and magnetic properties in a new family of molecular materials based on the organic donor BET-TTF and the perrhenate anion. *Journal of Materials Chemistry*, **2002**, 12, 432-441		7
195	Characterization of the Fermi surface of (BEDO-TTF)5[CsHg(SCN)4]2 by magnetoresistance measurements and tight-binding band structure calculations. *Journal of Materials Chemistry*, **2002**, 12, 483-488		13
194	Crystal and electronic structures of the radical cation salt based on EDT-TTF and the photochromic nitroprusside anion, (EDT-TTF)3[Fe(CN)5NO]. *Synthetic Metals*, **2002**, 128, 325-332	3.6	12
193	Molecular conductors based on radical cation hydrated halides: new crystal phase of the (BEDT-TTF)3Br2□2H2O organic metal. *Synthetic Metals*, **2002**, 131, 41-48	3.6	4

192	Possible nonactivated conductivity of the low-dimensional ternary nitride Ca(2)GeN(2). *Inorganic Chemistry*, **2002**, 41, 4630-2	5.1	2
191	Synthesis, electronic and crystal structure of a new organic semiconductor tetramethyltetrathiafulvalene-trinitroresorcinol (2:1), (TMTTF)2(C6H2N3O8). *Zeitschrift Fur Kristallographie - Crystalline Materials*, **2001**, 216, 623-628	1	2
190	Activation of C--H... Halogen (Cl, Br, and I) hydrogen bonds at the organic/inorganic interface in fluorinated tetrathiafulvalenes salts. *Chemistry - A European Journal*, **2001**, 7, 2635-43	4.8	34
189	Crystal and electronic structure of new organic semiconductors with rare-earth metal counter-anions. *Mendeleev Communications*, **2001**, 11, 182-183	1.9	3
188	Experimental and theoretical study of band structure of InSe and In1□GaxSe (x. *Physical Review B*, **2001**, 63,	3.3	64
187	Comparative study of BEDT-TTF and Ni(dddt) 2 electroconducting salts with the HXO 4 (X = Se, S) anions. *Synthetic Metals*, **2001**, 124, 357-362	3.6	8
186	Hal?Hal interactions in a series of three isostructural salts of halogenated tetrathiafulvalenes. Contribution of the halogen atoms to the HOMO□HOMO overlap interactions. *Journal of Materials Chemistry*, **2001**, 11, 1570-1575		84
185	Cation radical salts of cyano(ethylenedithio)tetrathiafulvalene with halogenated anions: annihilation of the CN□Hal interaction and stabilisation of conducting, antiferromagnetic square or chain-type salts. *New Journal of Chemistry*, **2001**, 25, 1418-1424	3.6	23
184	First-order phase transition in the organic metal □(BETS)2C(CN)3. *Journal of Materials Chemistry*, **2001**, 11, 332-336		3
183	Interplay between theory and experiment insolid state inorganic chemistry. *Journal of Materials Chemistry*, **2001**, 11, 1-10		14
182	Hybrid molecular materials based upon organic pi-electron donors and metal complexes. Radical salts of bis(ethylenethia)tetrathiafulvalene (BET-TTF) with the octahedral anions hexacyanoferrate(III) and nitroprusside. The first kappa phase in the BET-TTF family. *Inorganic Chemistry*, **2001**, 40, 3526-33	5.1	38
181	Halides of BET-TTF: Novel Hydrated Molecular Metals. *Advanced Materials*, **2000**, 12, 54-58	24	6
180	Donor Slab Robustness and Band Filling Variations in BDT□TTP-based Molecular Conductors: □(BDT□TTP)6[Re6S6Cl8]□(CH2Cl□CHCl2)2 and □(BDT□TTP)6 [Mo6Cl14]□(CH2Cl□CHCl2)2. *Advanced Materials*, **2000**, 12, 436-439	24	32
179	Crystal Structure and Coexistence of Localized and Delocalized Electrons in Nb12O29. *Journal of Solid State Chemistry*, **2000**, 149, 176-179	3.3	6
178	Electronic structure of the superconducting layered ternary nitrides CaTaN2 and CaNbN2. *Physical Review B*, **2000**, 62, 1512-1515	3.3	11
177	A new stable organic metal based on the BEDO-TTF donor and the doubly charged nitroprusside anion, (BEDO-TTF)4[Fe(CN)5NO]. *Journal of Materials Chemistry*, **2000**, 10, 2017-2023		25
176	Electronic structures of M21S8 (M = Nb, Zr) and (M,M')21S8 (M, M' = Hf, Ti; Nb, Ta) phases and reasons for variations in the metal site occupations. *Inorganic Chemistry*, **2000**, 39, 4200-5	5.1	2
175	An Efficient, Redox-Enhanced Pair of Hydrogen-Bond Tweezers for Chloride Anion Recognition, a Key Synthon in the Construction of a Novel Type of Organic Metal based on the Secondary Amide-Functionalized Ethylenedithiotetrathiafulvalene, □(EDT-TTF-CONHMe)2[Cl□H2O]. *Chemistry of Materials*, **2000**, 12, 1898-1904	9.6	71

174	. *Chemistry of Materials*, **2000**, 12, 2250-2256	9.6	12
173	Electronic structure of monoclinic TeMo5O16: Prediction of semiconducting behavior. *Physical Review B*, **2000**, 62, 16430-16434	3.3	5
172	Hybrid molecular materials based upon the photochromic nitroprusside complex, [Fe(CN)5NO]2-, and organic pi-electron donors. Synthesis, structure, and properties of the radical salt (TTF)7[Fe(CN)5NO]2 (TTF = tetrathiafulvalene). *Inorganic Chemistry*, **2000**, 39, 5394-7	5.1	29
171	Band structure and Fermi surface of the (BEDT-TTF)4M[Fe(CN)5NO]2 (M=Na, K, Rb,) molecular metals containing the photochromic nitroprusside anion. *Solid State Communications*, **1999**, 111, 329-333	1.6	25
170	Electronic structure of transition metal complex-based molecular metals and superconductors. *Coordination Chemistry Reviews*, **1999**, 185-186, 629-651	23.2	60
169	Covalent Linking of Slabs of EDT TTF Moieties: Bis(ethylenedithiotetrathiafulvalenyl)ethane and Its 1:1 Radical Cation Salt with Au(CN)2 *Advanced Materials*, **1999**, 11, 766-769	24	11
168	Te Te Interlayer Interactions, Te -g Metal Electron Transfer and Electrical Conductivity in the MM?Te5 Phases (M = Nb, M? = Ni, Pd; M = Ta, M? = Ni, Pt). *European Journal of Inorganic Chemistry*, **1999**, 1999, 1701-1706	2.3	2
167	The [(DT-TTF)2M(mnt)2] Family of Radical Ion Salts: From a Spin Ladder to Delocalised Conduction Electrons That Interact with Localised Magnetic Moments. *Chemistry - A European Journal*, **1999**, 5, 2025-2039	4.8	65
166	Directing the Structures and Collective Electronic Properties of Organic Conductors: The Interplay of Overlap Interactions and Hydrogen Bonds. *Chemistry - A European Journal*, **1999**, 5, 2971-2976	4.8	77
165	Organic metals based on BEDT-TTF and BEDO-TTF chlorides. *Synthetic Metals*, **1999**, 102, 1650-1653	3.6	4
164	Structural aspects of the phase transitions in (BEDO-TTF)2ReO4 H2O. *Synthetic Metals*, **1999**, 103, 1853-1856	3.6	7
163	The (DT-TTF)-M(mnt)2 Family of Compounds. *Synthetic Metals*, **1999**, 102, 1743-1746	3.6	11
162	New family of low-dimensional organic metals based on the asymmetrical multisulfur donor ETEDT-TTF: transport and magnetotransport properties. *Synthetic Metals*, **1999**, 102, 1772-1773	3.6	3
161	Fermi surface determination of (BEDO-TTF)2ReO4.H2O. *Synthetic Metals*, **1999**, 103, 1938-1939	3.6	2
160	Shubnikov-de haas oscillations in a new stable organic metal (BETS)2C(CN)3. *Synthetic Metals*, **1999**, 103, 1969-1970	3.6	1
159	Crystal Structure of the Host Lattices of the Superconductors LixMNX (M = Zr, Hf; X = Cl, Br). *Chemistry of Materials*, **1999**, 11, 203-206	9.6	40
158	A Remarkable Family of Rhodium Acetonitrile Compounds Spanning Three Oxidation States and with Nuclearities Ranging from Mononuclear and Dinuclear to One-Dimensional Chains. *Journal of the American Chemical Society*, **1999**, 121, 8005-8016	16.4	100
157	Chemical Transport Synthesis, Electrochemical Behavior, and Electronic Structure of Superconducting Zirconium and Hafnium Nitride Halides. *Inorganic Chemistry*, **1999**, 38, 4530-4538	5.1	22

156	Hydrogen Bonding and Transport Properties of Molecular Conductors **1999**, 337-351		
155	Electronic structure of the (BEDT-TTF)2MHg(XCN)4 (M = Tl, K, NH4; X = S, Se) molecular metals: on the 1D vs. 2D character of the charge carriers. *Computational and Theoretical Chemistry*, **1998**, 424, 135-143		
154	A new stable organic metal: -(BETS)C(CN). The first -type radical cation salt with a planar-triangular discrete organic anion. *European Physical Journal B*, **1998**, 5, 179-185	1.2	16
153	Crystal engineering and [C-H O] hydrogen bonds at the organic/inorganic interface. The bi-continuous hybrid composite, (2/3-3)-(EDT-TTF)8[Ca(H2O)4]2(TeW6O24)7H2O2. *Comptes Rendus De L'Academie Des Sciences - Series IIc: Chemistry*, **1998**, 1, 627-633		2
152	Concerning the first-order phase transition in the low-dimensional organic superconductor (BEDOTTF)2ReO4 H2O. Crystal and electronic band structures below the phase transition (T = 170 K). *European Physical Journal B*, **1998**, 1, 419-428	1.2	13
151	Low temperature crystal and electronic band structure of the (BEDOTTF)2Cl1.28(H3O)0.282.44H2O stable organic metal. *Journal of Materials Chemistry*, **1998**, 8, 1151-1156		7
150	Concerning the Resistivity Anomaly in the Layered Pnictide Oxide Na2Ti2Sb2O. *Inorganic Chemistry*, **1998**, 37, 5807-5810	5.1	26
149	Dimensionality and Fermi Surface of Low-Dimensional Metals *Chemistry of Materials*, **1998**, 10, 2770-2786	9.6	19
148	Structure and Physical Properties of a New 1:1 Cation-Radical Salt, (BEDTTTF)PF6. *Chemistry of Materials*, **1997**, 9, 1865-1877	9.6	18
147	Magnetic Properties and New Structural Classification of Molybdenum Phosphates Containing Mo(V). *Chemistry of Materials*, **1997**, 9, 68-75	9.6	30
146	Oxidation States, Transport Properties, and Te Te Short Contacts in the Ternary Transition Metal Tellurides Ta3Pd3Te14 and Ta4Pd3Te16. *Inorganic Chemistry*, **1997**, 36, 5050-5057	5.1	13
145	Origin of the Metal-to-Insulator Transition in H(0.33)MoO(3). *Inorganic Chemistry*, **1997**, 36, 4627-4632	5.1	22
144	Unusual transport and EPR properties of the (BET-TTF)-XF6 salts (X=P, As). *Synthetic Metals*, **1997**, 86, 1993-1994	3.6	8
143	Metallic conductivity in a disordered charge-transfer salt derived from cis-BET-TTF. *Synthetic Metals* , **1997**, 86, 2145-2146	3.6	12
142	Anisotropic thermopower in the charge density wave quasi two-dimensional compounds (PO2)4(WO3)2m(m=4, 6). *Synthetic Metals*, **1997**, 86, 2189-2190	3.6	2
141	Electronic Band Structure Study of the Transport Properties of the Intermetallic Compounds ZrRuP and ZrRuSi. *Inorganic Chemistry*, **1997**, 36, 6058-6063	5.1	15
140	An Organic Spin-Ladder Molecular Material. *Angewandte Chemie International Edition in English*, **1997**, 36, 2324-2326		48
139	Eine organische Verbindung mit Leiteranordnung der Spins. *Angewandte Chemie*, **1997**, 109, 2418-2421	3.6	5

138	Structure and Chemical Bonding in K14Cd9Tl21, a Compound Containing Both Isolated Tl7-11 Clusters and 2?[Cd9Tl7-10] Metallic Layers. *Chemistry - A European Journal*, **1997**, 3, 799-806	4.8	7
137	Electronic Structure of Layered Oxides Containing M(2)O(7) (M = V, Nb) Double Octahedral Slabs. *Inorganic Chemistry*, **1996**, 35, 1179-1184	5.1	12
136	Conducting thin films of molecular organic conductors, tetrathiafulvalene-7,7,8,8-tetracyano-p-quinodimethane (TTF-TCNQ). *Synthetic Metals*, **1996**, 76, 309-312	3.6	8
135	Metal Complexes of Dithiolate Ligands: 5,6-Dihydro-1,4-dithiin-2,3-dithiolato (dddt(2-)), 5,7-Dihydro-1,4,6-trithiin-2,3-dithiolato (dtdt(2-)), and 2-Thioxo-1,3-dithiole-4,5-dithiolato (dmit(2-)). Synthesis, Electrochemical Studies, Crystal and Electronic Structures, and Conducting Properties.	5.1	36
134	Electronic Structure of the $mathsf{alpha}$-(BEDT-TTF)$mathsf{_2}$MHg(XCN)$mathsf{_4}$ (M = Tl, K, NH$mathsf{_4}$; X = S, Se) and Related Phases. Synthesis and Crystal Structure of the New Stable Organic Metal $alpha$-(BEDT-TTF)$mathsf{_2}$TlHg(Se$mathsf{_{rm Me3TTFPO3H2, a Redox Phosphonic Acid and Its Monoanilinium Salt [PhNH+3][Me3TTFPO(OH)O-], the Electrocrystallized Neutral (Zwitterionic) Radical [Me3TTFPO(OH)O-]+, and Their Associated Lamellar Constructions in the Solid State. *Chemistry - A European Journal*, **1996**, 2, 1275-1282		29
133		4.8	29
132	Unprecedented Conversion of a Compound with Metal Metal Bonding into a Solvated Molecular Wire. *Angewandte Chemie International Edition in English*, **1996**, 35, 2772-2774		82
131	Preparation and characterization of conducting thin films of molecular organic conductors (TTF-TCNQ). *Journal of Crystal Growth*, **1996**, 166, 798-803	1.6	24
130	Stable Molecular Metal [Pd(dddt)2] Ag1.54Br3.50: Synthesis, Crystal Structure, Transport Properties and Electronic Band Structure. *Journal De Physique, I*, **1996**, 6, 1555-1565		14
129	Fermi Surface Nesting and Electronic Instabilities in Transition Metal Oxides and Bronzes. *NATO ASI Series Series B: Physics*, **1996**, 271-283		
128	Structural and Electronic Instabilities of Transition Metal Chalcogenides. *NATO ASI Series Series B: Physics*, **1996**, 285-302		6
127	Effect of the cooling rate on the transverse magnetoresistance of (TSeT)2Cl in its charge-density wave ground state. *Physica B: Condensed Matter*, **1995**, 211, 286-289	2.8	2
126	Structural and electronic properties of the one-dimensional organic metal bis(thiodimethylene)-tetrathiafulvalene tetracyanoquinodimethane. *Physical Review B*, **1995**, 52, 8747-8758	3.3	11
125	Structural and electronic properties of the molecular conductors (EDTTTF)x[Pd(dmit)2]y(x:y=2:3 and 2:2). *Journal of Physics Condensed Matter*, **1995**, 7, 4673-4695	1.8	11
124	Fermi-Surface Instabilities in the Organic Conductor (TMTSF) 2 NO 3 : High-Pressure Studies. *Europhysics Letters*, **1995**, 29, 635-640	1.6	12
123	Solution Chemistry of Chalcohalide Hexanuclear Rhenium Cluster Monoanions: Substitution Reactions and Structural and LSIMS Characterization of the Heterosubstituted Cluster Dianions, (n-Bu4N)2[Re6Q5ECl8] (Q = S, E = O, S, Se; Q = Se, E = S, Se, Te). *Inorganic Chemistry*, **1995**, 34, 5307-5313	5.1	42
122	A New Family of Molecular Metals Based on Bis(ethylenethio)tetrathiafulvalene (BET-TTF) and Octahedral Counterions. *Chemistry of Materials*, **1995**, 7, 1558-1567	9.6	23
121	Cooling rate dependence of the lattice parameters of (TMTSF)2ClO4. *Synthetic Metals*, **1995**, 70, 761-762	3.6	3

120	Two-band systems and hidden nesting: Novel aspects of the electronic structure of low-dimensional metals. *Synthetic Metals*, **1995**, 70, 1009-1012	3.6	7
119	Weak electron correlations and charge-density waves in TTF[M(dmit)2]2, with M = Ni, Pd. *Synthetic Metals*, **1995**, 70, 1045-1046	3.6	1
118	Interplay between structural, magnetic properties and calculated band structures of (EDT-TTF)2[M(dmit)2]2 where M = Ni, Pd. *Synthetic Metals*, **1995**, 70, 1063-1064	3.6	4
117	Magnetoresistance in pulsed fields, band structure calculations and charge-density wave instability in (TSeT)2Cl. *Synthetic Metals*, **1995**, 70, 1279-1280	3.6	4
116	Electronic properties of isostructural organic conductors (ET)3(HSO4)2 and [Ni(dddt)2]3(HSO4)2. Thermopower and tight-binding calculations. *Synthetic Metals*, **1995**, 71, 1867-1868	3.6	3
115	The M(dddt)2 family of conducting complexes: [Ni(dddt)2]3(AuBr2)2, the first quasi-two-dimensional metal stable down to at least 1.3 K. *Journal of Materials Chemistry*, **1995**, 5, 1633		21
114	Organic□inorganic molecular aggregates and their association within long-range ordered crystalline assemblies: relevance to the template effect in solid-state chemistry. *Journal of Materials Chemistry* , **1995**, 5, 1707-1718		27
113	Control of the dimensionality of the Fermi surface of metallic monolayers by chemisorption. *Journal of Chemical Physics*, **1995**, 103, 6283-6289	3.9	1
112	Bis(ethylenethio)tetrathiafulvalene (BET-TTF), an organic donor with high electrical conductivity. *Advanced Materials*, **1995**, 7, 1023-1027	24	21
111	KNiPS4: A New Thiophosphate with One- and Two-Dimensional Structural Arrangements. *Journal of Solid State Chemistry*, **1995**, 116, 107-112	3.3	26
110	Stabilized 1D Metal in TTF(Ni(dmit)2)2through Very Weak Coupling between Phonons and Weakly Correlated Fermions. *Acta Physica Polonica A*, **1995**, 87, 781-784	0.6	3
109	Magnetoresistance Studies in the Low-Dimensional Organic Metal □(ET)2TlHg(SeCN)4 under Pressure: Experiments and Simulation by Tight Binding Band Structure Calculations. *Journal De Physique, I*, **1995**, 5, 1301-1310		10
108	Concerning the first-order transition in the ?-phase (BEDT-TTF)4PtCl6 . C6H5CN. *Journal De Physique, I*, **1994**, 4, 1479-1490		20
107	Comparison of the electronic structures of isostructural (BEDT-TTF)3(HSO4)2 and [Ni(dddt)2] 3(HSO4)2 molecular metals. *Journal De Physique, I*, **1994**, 4, 1439-1450		8
106	(TMTTF)2Br: The First Organic Superconductor in the (TMTTF)2X family. *Advanced Materials*, **1994**, 6, 762-765	24	16
105	Electronic Structure of the 1:1 Mixed Molecular and Polymeric Conductor (perylene)Co(mnt)2(CH2Cl2)0.5 and Comparison with the 2:1 .alpha.-(perylene)2M(mnt)2 Phases. *Inorganic Chemistry*, **1994**, 33, 4290-4294	5.1	19
104	Preparation, crystal structures, conductivities and electronic structures of [et]3[NiCl4]□H2O and [et]3[AuBr4][et = bis(ethylenedithio)tetrathiafulvalene]. *Journal of the Chemical Society Dalton Transactions*, **1994**, 1995-2004		11
103	Structure-Property Correlations in the Platinum Oxide and Palladium Sulfide Bronzes with Columnar Chains of Square-Planar TX4 Units (T = Pt, X = O; T = Pd, X = S). *Journal of the American Chemical Society*, **1994**, 116, 2115-2120	16.4	14

102	Analysis of the partially-filled d-block band of the layered metal lanthanum diiodide and probable cause for the absence of structural instability. *Inorganic Chemistry*, **1994**, 33, 287-291	5.1	4
101	Possibility of Charge Density Wave Instability in the Barium Tungsten Bronze Ba0.15WO3. *Inorganic Chemistry*, **1994**, 33, 1864-1868	5.1	2
100	Synthesis, Crystal Structure, Electrical Properties and Electronic Band Structure of (NHyMe4-y)x[M(dmit)2] Complexes (M = Ni, Pd, Pt; dmit2- = 2-Thioxo-1,3-dithiole-4,5-dithiolato). *Inorganic Chemistry*, **1994**, 33, 3401-3414	5.1	38
99	Superconductivity and magnetic field induced spin density waves in the (TMTTF)2X family. *Journal De Physique, I*, **1994**, 4, 1539-1549		42
98	Characterization of the Fermi surface of BEDT-TTF4[Hg2Cl6] .PhCl by electronic band structure calculations. *Journal De Physique, I*, **1994**, 4, 939-947		14
97	Isotope effect in superconductivity on 13C substituted β-(BEDT-TTF)2I3. *Synthetic Metals*, **1993**, 56, 2542-2547	3.6	5
96	STRUCTURAL AND ELECTRONIC ORIGIN OF THE HIDDEN NESTING AND CHARGE DENSITY WAVES IN TRANSITION METAL OXIDES AND BRONZES. *International Journal of Modern Physics B*, **1993**, 07, 4005-4043	1.1	36
95	Importance of the interlayer Te...Te contacts on the electronic structure of the layered niobium germanium telluride Nb3Ge0.9Te6. *Inorganic Chemistry*, **1993**, 32, 10-12	5.1	13
94	Structural and electronic study of donors composed of two TTF moieties linked by tellurium bridges. *Chemistry of Materials*, **1993**, 5, 1199-1203	9.6	21
93	Nature of the charge density wave images of layered tantalum dichalcogenides 1T-TaX2 (X = sulfur, selenium) in scanning tunneling and atomic force microscopy. *Journal of the American Chemical Society*, **1993**, 115, 3760-3765	16.4	30
92	Hydrogen-bond tuning of macroscopic transport properties from the neutral molecular component site along the sries of metallic organic-inorganic solvates (BEDT-TTF)4Re6Se5Cl9.[guest], [guest = DMF, THF, dioxane]. *Journal of the American Chemical Society*, **1993**, 115, 4101-4112	16.4	102
91	Bis- and tetrakis(1,4-dithiafulven-6-yl)-substituted tetrathiafulvalenes and dihydrotetrathiafulvalenes: a novel class of planar donor molecules with multiple redox functionalities and the demonstration of a novel type of two-dimensional association in the solid state. *Chemistry of Materials*, **1993**, 5, 1196-1198	9.6	37
90	Bis and tetrakis (1,4-dithiafulven-6-yl) substituted tetrathiafulvalenes (TTF) and dihyrdro-TTF as precursors of organic metals of enhanced dimensionality. *Synthetic Metals*, **1993**, 56, 2132-2135	3.6	3
89	(BTDM-TTF)-TCNQ complex, a new organic metal. *Synthetic Metals*, **1993**, 56, 2050-2056	3.6	5
88	Inhibited superconductivity induced by localization effects in (EDT-TTF)2[Pd(dmit)2]2. *Synthetic Metals*, **1993**, 56, 2833-2838	3.6	5
87	Magnetic susceptibility of tetrathiafulvalene. *Physical Review B*, **1993**, 47, 1647-1650	3.3	12
86	Structural Origin of the Semiconducting Properties of Sb4Mo20O62. *Journal of Solid State Chemistry*, **1993**, 105, 434-443	3.3	2
85	Factors affecting the metallic versus semiconducting properties of charge transfer salts containing [M(dddt)2]2 and [M(dmit)2]2 (M = Pd, Pt) dimers. *Solid State Communications*, **1993**, 88, 699-703	1.6	22

84	Isotope effect in the organic superconductor κ-(BEDT-TTF)2I3 where BEDT-TTF is bis (ethylenedithiotetrathiafulvalene). *Journal De Physique, I*, **1993**, 3, 871-885		9
83	Comparison of the electronic structures of the BEDT-TTF4[M(CN)4] (M = Ni, Pt) and BEDT-TTF4[M(C2O4)2] (M = Pt, Cu) salts. Structural requirements for hidden Fermi surface nesting. *Journal De Physique, I*, **1993**, 3, 2451-2461		4
82	Analogies between the concepts of molecular chemistry and solid-state physics concerning structural instabilities. Electronic origin of the structural modulations in layered transition metal dichalcogenides. *Journal of the American Chemical Society*, **1992**, 114, 9587-9600	16.4	192
81	Molecular interactions, band structure, and BEDT-TTF oxidation states in the molecular conductor (BEDT-TTF)3[V(dmit)3]2. *Inorganic Chemistry*, **1992**, 31, 3176-3178	5.1	11
80	Some general conditions for hidden Fermi surface nesting. *Inorganic Chemistry*, **1992**, 31, 4169-4173	5.1	27
79	Nonelectronic origin of superlattice modulations and resistivity anomalies in ternary copper sulfides. *Solid State Communications*, **1992**, 81, 895-899	1.6	25
78	Electronic structure and properties of anionic mixed valence and layered CrTe3: The question of extended tellurium bonding in transition metal tellurides. *Journal of Solid State Chemistry*, **1992**, 98, 59-70	3.3	25
77	Importance of short interlayer Te···Te contacts for the structural distortions and physical properties of CdI2-type layered transition-metal ditellurides. *Journal of Solid State Chemistry*, **1992**, 99, 189-199	3.3	86
76	A construction principle of the β-phase based on the efficient (O?H)donor–anion structural functionality: The examples of β-(EDTTTF(CH2OH))2X (X = ClO and ReO). *Advanced Materials*, **1992** , 4, 579-581	24	54
75	One-dimensional physics in organic conductors (TMDTDSF)2X, X = PF6, ReO4 : 77Se-NMR experiments. *Journal De Physique, I*, **1992**, 2, 677-694		12
74	Antiperovskite Structure with Ternary Tetrathiafulvalenium Salts: Construction, Distortion, and Antiferromagnetic Ordering. *Angewandte Chemie International Edition in English*, **1991**, 30, 1498-1500		43
73	Structural and electronic properties of Cs(Pd(dmit)2)2. *Journal of Physics Condensed Matter*, **1991**, 3, 933-954	1.8	40
72	Structural instabilities and electronic structures of the D(M(dmit)2)2 molecular conductors and superconductors. *Synthetic Metals*, **1991**, 42, 2191-2194	3.6	6
71	(TMTSF)3Ta2F11: Synthesis, structural chemistry, electronic structure and physical properties. *Synthetic Metals*, **1991**, 42, 1939-1942	3.6	6
70	Role of large but defective deltahedra in the structural chemistry of very complex solid borides and gallides. *Inorganic Chemistry*, **1991**, 30, 1991-1998	5.1	32
69	Charge-density-wave instabilities expected in monophosphate tungsten bronzes. *Physical Review B*, **1991**, 43, 1894-1902	3.3	47
68	Conceptual aspects of structure-property correlations and electronic instabilities, with applications to low-dimensional transition-metal oxides. *Chemical Reviews*, **1991**, 91, 965-1034	68.1	254
67	Interplay between charge density waves and reentrant superconductivity in the pressure – temperature phase diagram of TTF(Ni(dmit)2)2. *Synthetic Metals*, **1991**, 43, 3841-3844	3.6	4

66	Hidden fermi surface nesting and charge density wave instability in low-dimensional metals. *Science* , **1991**, 252, 96-8	33.3	161
65	On the possible electronic instability of the monophosphate tungsten bronze (WO3)4(PO2)4. *Journal of Solid State Chemistry*, **1990**, 86, 131-134	3.3	10
64	Concerning the band structure of D(M(dmit)2)2 (D=TTF,Cs,NMe4); M=Ni,Pd) molecular conductors and superconductors: Role of the M(dmit)2 Homo and Lumo. *Solid State Communications*, **1990**, 75, 633-638	1.6	82
63	Semimetallic versus semiconducting properties of MX2 layer compounds containing d2 metal ions. *Inorganic Chemistry*, **1990**, 29, 1398-1401	5.1	18
62	Regioselectivity of radical attacks on substituted olefins. Application of the state-correlation-diagram (SCD) model. *Journal of the American Chemical Society*, **1990**, 112, 1446-1452	16.4	71
61	Comparison of the electronic structures of layered transition-metal trichalcogenides thallium triselenide, thallium trisulfide and niobium triselenide. *Inorganic Chemistry*, **1990**, 29, 1401-1407	5.1	47
60	Similarity of the electronic properties of the monophosphate tungsten bronzes. *Inorganic Chemistry* , **1990**, 29, 3871-3875	5.1	15
59	Fused and linked deltahedral clusters in the chemistry of the Group 13 elements. *Journal of the American Chemical Society*, **1990**, 112, 7207-7217	16.4	45
58	Band electronic structure study of the structural modulation in the Magneli phase molybdenum oxides, Mo8O23. *Inorganic Chemistry*, **1990**, 29, 2256-2260	5.1	16
57	Apparent absence of electronic instability in the one-dimensional metal sodium copper sulfide (Na3Cu4S4). *Inorganic Chemistry*, **1990**, 29, 1395-1397	5.1	18
56	Novel redox properties of the paramagnetic hexanuclear niobium cluster halide Nb6Cl183- and the preparation, structures, and conducting and magnetic properties of its one-dimensional mixed-valence tetramethyltetra(selena and thia)fulvalenium salts: [TMTSF and TMTTF]5[Nb6Cl18].cntdot.(CH2Cl2)0.5. *Chemistry of Materials*, **1990**, 2, 123-132	9.6	26
55	Temperature dependent locally resolved 13C Knight shifts in the organic conductor TTF[Ni(dmit)2]2. *Journal De Physique*, **1990**, 51, 2465-2476		15
54	Electronic instabilities of the quasi-two-dimensional monophosphate tungsten bronze P4W12O44. *Physical Review B*, **1989**, 39, 12969-12972	3.3	43
53	Quasi-two-dimensional electronic properties of the monophosphate tungsten bronzes NaxP4W8O32 and NaxP4W12O44: Crystal growth, physical properties, and electronic band structure. *Journal of Solid State Chemistry*, **1989**, 81, 173-180	3.3	15
52	Anisotropic electronic properties of the diphosphate tungsten bronzes K2P8W24O88, K2P8W28O100 and their substituted compounds. *Journal of Solid State Chemistry*, **1989**, 80, 266-275	3.3	8
51	Energy factors governing the partial irreversibility of lithium intercalation in layered trichalcogenides MX3 (M = Ti, Zr, Hf; X = S, Se) and the structural changes in the intercalated species Li3MX3. *Inorganic Chemistry*, **1989**, 28, 3043-3047	5.1	12
50	Origin of metal clustering in transition-metal chalcogenide layers MX2 (M = Nb, Ta, Mo, Re; X = S, Se). *Journal of the American Chemical Society*, **1989**, 111, 3778-3782	16.4	32
49	Structural origin of semiconducting properties of the molybdenum red bronzes A0.33MoO3 (A = potassium, rubidium, cesium, thallium). *Inorganic Chemistry*, **1989**, 28, 267-271	5.1	11

48	Crystal symmetry governing the metallic vs semiconducting properties of cesium molybdenum bronzes CsxMoO3 (x .simeq. 0.25, 0.33). *Inorganic Chemistry*, **1989**, 28, 1609-1610	5.1	7
47	Structural and electronic origin of the three-dimensional electrical properties of tungsten oxyphosphate, P8W12O52, and its inserted and substituted analogs AxP8W12O52 (A = Li, Na) and P8W12-xMoxO52. *Inorganic Chemistry*, **1989**, 28, 2455-2459	5.1	4
46	Band electronic structure study of the electronic instability in the Magneli phase molybdenum oxide [Mo4O11]. *Inorganic Chemistry*, **1989**, 28, 1466-1472	5.1	59
45	Resitivity anomalies of the diphosphate tungsten bronze Cs1-xP8W8O40(x = 0-0.46) and its partially substituted phases CsxAyP8W8O40 (A = Rb, Na) and CsP8W8-xMoxO40: synthesis, physical property measurements, and band electronic structure calculations. *Inorganic Chemistry*, **1989**, 28, 2451-2455	5.1	8
44	A theoretical study of models for X2Y2 Zintl ions. *Journal of the American Chemical Society*, **1989**, 111, 8105-8111	16.4	17
43	Chemical bonding and electronic instability in molybdenum oxide metals. *Accounts of Chemical Research*, **1989**, 22, 375-381	24.3	24
42	On the band electronic structure of X [M (dmit)2]2 (X = TTF, (CH3)4N ; M = Ni, Pd) molecular conductors and superconductors. *Journal De Physique*, **1989**, 50, 2967-2981		132
41	Semiconducting properties of lithium molybdate, Li0.33MoO3. *Inorganic Chemistry*, **1988**, 27, 228-232	5.1	15
40	Band electronic structure study of the semimetallic properties and the anisotropic resistivity hump in zirconium tritelluride. *Journal of the American Chemical Society*, **1988**, 110, 104-108	16.4	34
39	Linear electron-hole-electron pair model of high-temperature superconductivity in La2-xMxCuO4 and LBa2Cu3O7-y. Small Cooper pair formation in linear Cu2+-O-Cu3+-O-Cu2+ units via concerted breathing-mode vibration. *Inorganic Chemistry*, **1988**, 27, 2394-2396	5.1	3
38	Theoretical analysis of the rearrangement and inversion processes in oxiranyl radicals. *Computational and Theoretical Chemistry*, **1988**, 168, 93-104		1
37	Chromium boride (CrB4) and manganese boride (MnB4): electronic structures of two unusual systems containing the tetragonal carbon net. *Inorganic Chemistry*, **1988**, 27, 4437-4444	5.1	34
36	Band electronic structure of the lithium molybdenum purple bronze Li0.9Mo6O17. *Journal of the American Chemical Society*, **1988**, 110, 358-363	16.4	54
35	X-Ray and Theoretical Study of Cyclophane-tetracyanoethylene Charge Transfer Complexes. *Molecular Crystals and Liquid Crystals Incorporating Nonlinear Optics*, **1988**, 164, 179-195		
34	Metallic versus nonmetallic properties of ternary chalcogenides: tantalum metal selenide, Ta2MSe7 (M = nickel, platinum), and tantalum nickel chalcogenide, Ta2NiX5 (X = sulfide, selenide). *Inorganic Chemistry*, **1987**, 26, 3974-3976	5.1	32
33	Potentially conducting organometallic systems: the stibaphenalenyl series. *Inorganic Chemistry*, **1987**, 26, 3797-3802	5.1	9
32	Band electronic structure of the purple potassium molybdenum bronze K0.9Mo6O17. *Journal of the American Chemical Society*, **1987**, 109, 6308-6313	16.4	43
31	Charge density wave as a probable cause for the phase transition at 125 K in the ternary molybdenum oxide La2Mo2O7. *Inorganic Chemistry*, **1987**, 26, 842-844	5.1	8

30	On the electronic structure of MPS3 phases. *Inorganic Chemistry*, **1987**, 26, 963-965	5.1	39
29	Electronic structure of Nb3X4 type compounds. *Inorganic Chemistry*, **1986**, 25, 1488-1491	5.1	23
28	Symmetry control of the coloring problem: the electronic structure of MB2C2 (M = calcium, lanthanum, ...). *Journal of the American Chemical Society*, **1986**, 108, 3971-3976	16.4	54
27	The unusual structural feature of binuclear platinum chains [Pt2(L-L)4X]n-.infin.. *Inorganic Chemistry* , **1986**, 25, 1726-1728	5.1	11
26	Electronic structure of transition-metal borides with the AlB2 structure. *Journal of the American Chemical Society*, **1986**, 108, 6561-6568	16.4	89
25	Theoretical analysis of radical reactions: on the anomalous behavior of methyl toward fluoro-substituted olefins. *The Journal of Physical Chemistry*, **1985**, 89, 4856-4861		24
24	MINDO/3 calculations on enthalpy and entropy effects in the cyclization of the hex-5-enyl, 2-methylhex-5-enyl, and 5-methylhex-5-enyl radicals. *Journal of the Chemical Society Perkin Transactions II*, **1985**, 1331		8
23	Extended polymetallic sandwich compounds. *Organometallics*, **1985**, 4, 805-815	3.8	63
22	Symmetry constraints to the electrical conductivity of partially oxidized stacks of metal bis(dioximates). *Solid State Communications*, **1984**, 50, 141-144	1.6	8
21	Theoretical analysis of bonding in monomeric and polymeric C5H5M compounds. *Organometallics*, **1984**, 3, 759-764	3.8	63
20	Theoretical study of the electrical behavior of one-dimensional metallophthalocyanines and related metallomacrocyclic compounds. *Inorganic Chemistry*, **1984**, 23, 573-579	5.1	70
19	Electronic switching of ring orientation in cyclopentadienyl-bridged polymers. *Inorganic Chemistry*, **1984**, 23, 2435-2440	5.1	7
18	Theoretical analysis of kinetic isotope effects. Deuterium isotope effects in the reaction of methyl with methane. *The Journal of Physical Chemistry*, **1984**, 88, 3545-3549		12
17	On the stability of [furan].+ and [vinylketene].+. *Journal of Molecular Structure*, **1983**, 94, 193-195	3.4	
16	Concerning the orientation in free radical additions to olefins. *Canadian Journal of Chemistry*, **1983**, 61, 2068-2069	0.9	17
15	Structure and stability of one-dimensional (MX2)n polymers. A band structure analysis. *Inorganic Chemistry*, **1983**, 22, 3856-3861	5.1	6
14	Polymeric one-dimensional [CoXL2]n vs. dimeric [CoXL2]2. Theoretical analysis of the factors favoring each form. *Inorganic Chemistry*, **1983**, 22, 2398-2401	5.1	8
13	Theoretical study of the addition of vinyl and cyclopropyl radicals to ethylene. *Journal of Organic Chemistry*, **1983**, 48, 4696-4700	4.2	4

12	On the stability of [Furan]⊟+ and [Vinylketene]⊟+. *Computational and Theoretical Chemistry*, **1983**, 94, 193-195		1
11	Theoretical analysis of kinetic isotope effects. The secondary deuterium effects in the addition of methyl radical to ethylene. *The Journal of Physical Chemistry*, **1983**, 87, 424-429		10
10	A molecular orbital interpretation of the structure of some halogenoalkyl radicals. *Journal of the Chemical Society Perkin Transactions II*, **1982**, 1217		5
9	Electronic origin of the thermochromic effect in 2,2',5,5'-tetramethylbistibole. *Journal of the American Chemical Society*, **1982**, 104, 3876-3879	16.4	41
8	A comment on SCF energy partitioning schemes. *Theoretica Chimica Acta*, **1981**, 60, 299-302		9
7	A qualitative molecular orbital picture of 2-substituted carbonyl derivatives of furan and pyrrole. *Journal of Heterocyclic Chemistry*, **1981**, 18, 1055-1056	1.9	9
6	Bond cleavage of the solvated methyl chloride anion: a primary electrochemical event. *Journal of the American Chemical Society*, **1980**, 102, 855-857	16.4	36
5	A theoretical study of benzene protonation. *Journal of the Chemical Society Perkin Transactions II*, **1979**, 1486-1489		11
4	La regle d'alder generalisee. *Tetrahedron*, **1978**, 34, 2283-2288	2.4	12
3	Theoretical study of the intramolecular hydrogen bonding in benzene derivatives. *Advances in Molecular Relaxation and Interaction Processes*, **1978**, 12, 265-287		22
2	The role of intermediate complexes in benzofuran protonations. *Journal of the Chemical Society Perkin Transactions II*, **1976**, 1789-1791		2
1	Analysis of high molecular weight esters and ketones in thymus. *Microchemical Journal*, **1975**, 20, 154-164	4.8	