

# Karoly Nemeth

## List of Publications by Year in descending order

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46  
papers

820  
citations

430874

18  
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501196

28  
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47  
docs citations

47  
times ranked

873  
citing authors

#	ARTICLE	IF	CITATIONS
1	Radical anion functionalization of two-dimensional materials as a means of engineering simultaneously high electronic and ionic conductivity solids. <i>Nanotechnology</i> , 2021, 32, 245709.	2.6	2
2	Li <sub>3</sub> BN <sub>2</sub> as a Transition Metal Free, High Capacity Cathode for Li-ion Batteries. <i>ChemElectroChem</i> , 2019, 6, 320-325.	3.4	9
3	On the synthesis of lithium boron nitride (Li <sub>3</sub> BN <sub>2</sub> ). <i>Ceramics International</i> , 2018, 44, 7734-7740.	4.8	6
4	Simultaneous oxygen and boron trifluoride functionalization of hexagonal boron nitride: a designer cathode material for energy storage. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	1.4	7
5	Metallic and semiconducting 1D conjugated polymers based on $\text{[S-C}_{\text{equiv}}\text{C]}$ repeating units in poly(sulfur acetylide). <i>Highlights in Theoretical Chemistry</i> , 2016, , 199-204.	0.0	0
6	Experimental and theoretical investigations of functionalized boron nitride as electrode materials for Li-ion batteries. <i>RSC Advances</i> , 2016, 6, 27901-27914.	3.6	27
7	Metallic and semiconducting 1D conjugated polymers based on $\text{[S-C}_{\text{equiv}}\text{C]}$ repeating units in poly(sulfur acetylide). <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	1.4	0
8	The synthesis of ternary acetylides with tellurium: Li <sub>2</sub> TeC <sub>2</sub> and Na <sub>2</sub> TeC <sub>2</sub> . <i>RSC Advances</i> , 2015, 5, 55986-55993.	3.6	3
9	Ultrahigh energy density Li-ion batteries based on cathodes of 1D metals with $\text{[Li-N-B]}$ repeating units in $\text{Li}_{1-x}\text{BN}_2$ ( $1 \leq x \leq 3$ ). <i>Journal of Chemical Physics</i> , 2014, 141, 054711.	3.0	11
10	Metal-Insulator Photocathode Heterojunction for Directed Electron Emission. <i>Physical Review Letters</i> , 2014, 112, 067601.	7.8	12
11	Materials design by quantum-chemical and other theoretical/computational means: Applications to energy storage and photoemissive materials. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 1031-1035.	2.0	7
12	CO <sub>2</sub> /oxalate cathodes as safe and efficient alternatives in high energy density metal-air type rechargeable batteries. <i>RSC Advances</i> , 2014, 4, 1879-1885.	3.6	19
13	Searching for low-workfunction phases in the Cs-Te system: The case of Cs <sub>2</sub> Te <sub>5</sub> . <i>Journal of Applied Physics</i> , 2013, 113, 183703.	2.5	3
14	Anomalous work function anisotropy in ternary acetylides. <i>Physical Review B</i> , 2012, 86, .	3.2	14
15	Efficient simultaneous reverse Monte Carlo modeling of pair-distribution functions and extended x-ray-absorption fine structure spectra of crystalline disordered materials. <i>Journal of Chemical Physics</i> , 2012, 136, 074105.	3.0	16
16	Theoretical Design of High-Brightness Photocathodes Based on Ultrathin Surface Layers on Metals and on Nanostructures. , 2010, , .		0
17	The choice of internal coordinates in complex chemical systems. <i>Journal of Computational Chemistry</i> , 2010, 31, 2078-2086.	3.3	6
18	High-Brightness Photocathodes through Ultrathin Surface Layers on Metals. <i>Physical Review Letters</i> , 2010, 104, 046801.	7.8	26

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19	Trace correcting density matrix extrapolation in self-consistent geometry optimization. <i>Journal of Chemical Physics</i> , 2010, 132, 124104.	3.0	3
20	Laser-Driven Coherent Betatron Oscillation in a Laser-Wakefield Cavity: Formation of Sinusoid Beam Shapes and Coherent Trajectories. , 2009, , .		2
21	Laser-Driven Coherent Betatron Oscillation in a Laser-Wakefield Cavity. <i>Physical Review Letters</i> , 2008, 100, 095002.	7.8	92
22	Beam slowing down in a laser plasma accelerator by laser-induced betatron oscillation. , 2008, , .		0
23	Electron injection by a nanowire in the bubble regime. <i>Physics of Plasmas</i> , 2007, 14, 053115.	1.9	36
24	First-principles isomer-specific absorption spectra of Ag11. <i>Physical Review B</i> , 2007, 75, .	3.2	28
25	Calculation of Vibrational Spectra of Linear Tetrapyrroles. 3. Hydrogen-Bonded Hexamethylpyrromethene Dimers. <i>Journal of Physical Chemistry A</i> , 2005, 109, 2139-2150.	2.5	20
26	Geometry optimization of crystals by the quasi-independent curvilinear coordinate approximation. <i>Journal of Chemical Physics</i> , 2005, 123, 194112.	3.0	7
27	The quasi-independent curvilinear coordinate approximation for geometry optimization. <i>Journal of Chemical Physics</i> , 2004, 121, 2877-2885.	3.0	21
28	An efficient method for the coordinate transformation problem of massively three-dimensional networks. <i>Journal of Chemical Physics</i> , 2001, 114, 9747-9753.	3.0	18
29	Linear scaling density matrix search based on signmatrices. <i>Journal of Chemical Physics</i> , 2000, 113, 6035-6041.	3.0	43
30	Linear scaling algorithm for the coordinate transformation problem of molecular geometry optimization. <i>Journal of Chemical Physics</i> , 2000, 113, 5598-5603.	3.0	27
31	Calculation of the Vibrational Spectra of Linear Tetrapyrroles. 2. Resonance Raman Spectra of Hexamethylpyrromethene Monomers. <i>Journal of Physical Chemistry B</i> , 2000, 104, 10885-10899.	2.6	27
32	Interpretation of the resonance Raman spectra of linear tetrapyrroles based on DFT calculations. <i>Chemical Physics Letters</i> , 1999, 311, 479-484.	2.6	38
33	Calculation of Vibrational Spectra of Linear Tetrapyrroles. 1. Global Sets of Scaling Factors for Force Fields Derived by ab Initio and Density Functional Theory Methods. <i>Journal of Physical Chemistry A</i> , 1999, 103, 289-303.	2.5	39
34	Vibrational analysis of model compounds for the tetrapyrrole chromophore in phytochrome. , 1999, , 171-172.		0
35	Triplet State Characteristics of Higher Fullerenes. <i>Journal of Physical Chemistry A</i> , 1998, 102, 1261-1273.	2.5	26
36	Triplet State Characteristics of Smaller Fullerenes. <i>Fullerenes, Nanotubes, and Carbon Nanostructures</i> , 1997, 5, 355-373.	0.6	2

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37	On The Differences Between Neutral and Negatively Charged C60Dimers. Fullerenes, Nanotubes, and Carbon Nanostructures, 1997, 5, 429-442.	0.6	1
38	Zero-field splitting of the lowest excited triplet state in thiophene oligomers. An experimental and theoretical investigation. Synthetic Metals, 1997, 84, 607-608.	3.9	8
39	Energetics and zero-field-splitting in triplet states of C70. Computational and Theoretical Chemistry, 1997, 398-399, 293-300.	1.5	7
40	Excited states of the C60 dimer. Synthetic Metals, 1996, 77, 107-110.	3.9	9
41	Zero-field-splitting in the lowest triplet state of C60. Chemical Physics Letters, 1996, 251, 115-118.	2.6	37
42	Structure and energetics of neutral and negatively charged C60 dimers. Chemical Physics Letters, 1996, 256, 119-125.	2.6	63
43	Zero-field-splitting and electron spin densities in the lowest excited triplet state of oligothiophenes. Journal of Chemical Physics, 1996, 105, 4441-4447.	3.0	34
44	Band structures of neutral and doped (C60) <sub>x</sub> polymers. Solid State Communications, 1994, 92, 407-411.	1.9	34
45	Electronic excitations in fullerenes: Jahn-Teller distorted structures of C60. Computational and Theoretical Chemistry, 1994, 311, 55-68.	1.5	27
46	Quinoid-aromatic competition as a tool for band structure design for conjugated polymers. Synthetic Metals, 1993, 57, 4260-4265.	3.9	3