## Ante Bilic

List of Publications by Year in descending order

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ANTE RILIC

#	Article	IF	CITATIONS
1	Direct connection of an amine to oligothiophene to generate push-pull chromophores for organic photovoltaic applications. Dyes and Pigments, 2019, 162, 315-323.	2.0	3
2	An efficient non-fullerene acceptor based on central and peripheral naphthalene diimides. Chemical Communications, 2018, 54, 5062-5065.	2.2	27
3	A Triphenylamine–Naphthalenediimide–Fullerene Triad: Synthesis, Photoinduced Charge Separation and Solutionâ€Processable Bulk Heterojunction Solar Cells. Asian Journal of Organic Chemistry, 2018, 7, 220-226.	1.3	12
4	Oxygen diffusion in the Ti3X alloys with elements from the IIIA or IVA groups and stability of their DO19crystal structure. Journal of Applied Physics, 2017, 121, 025105.	1.1	1
5	An H-shaped, small molecular non-fullerene acceptor for efficient organic solar cells with an impressive open-circuit voltage of 1.17 V. Materials Chemistry Frontiers, 2017, 1, 1600-1606.	3.2	30
6	Cyanopyridone flanked the tetraphenylethylene to generate an efficient, three-dimensional small molecule non-fullerene electron acceptor. Materials Chemistry Frontiers, 2017, 1, 2511-2518.	3.2	25
7	Donor–acceptor–acceptor-based non-fullerene acceptors comprising terminal chromen-2-one functionality for efficient bulk-heterojunction devices. Dyes and Pigments, 2017, 146, 502-511.	2.0	22
8	Machine learning and genetic algorithm prediction of energy differences between electronic calculations of graphene nanoflakes. Nanotechnology, 2017, 28, 38LT03.	1.3	19
9	Enhancing the efficiency of solution-processable bulk-heterojunction devices via a three-dimensional molecular architecture comprising triphenylamine and cyanopyridone. Dyes and Pigments, 2017, 137, 126-134.	2.0	10
10	A four-directional non-fullerene acceptor based on tetraphenylethylene and diketopyrrolopyrrole functionalities for efficient photovoltaic devices with a high open-circuit voltage of 1.18 V. Chemical Communications, 2016, 52, 8522-8525.	2.2	65
11	Graphene-like Two-Dimensional Ionic Boron with Double Dirac Cones at Ambient Condition. Nano Letters, 2016, 16, 3022-3028.	4.5	222
12	Naphthalene diimide-based non-fullerene acceptors for simple, efficient, and solution-processable bulk-heterojunction devices. RSC Advances, 2016, 6, 38703-38708.	1.7	17
13	Substantial Band-Gap Tuning and a Strain-Controlled Semiconductor to Gapless/Band-Inverted Semimetal Transition in Rutile Lead/Stannic Dioxide. ACS Applied Materials & Interfaces, 2016, 8, 25667-25673.	4.0	18
14	Twoâ€Dimensional Boron Hydride Sheets: High Stability, Massless Dirac Fermions, and Excellent Mechanical Properties. Angewandte Chemie, 2016, 128, 10448-10451.	1.6	94
15	Twoâ€Dimensional Boron Hydride Sheets: High Stability, Massless Dirac Fermions, and Excellent Mechanical Properties. Angewandte Chemie - International Edition, 2016, 55, 10292-10295.	7.2	100
16	Anomalous Enhancement of Mechanical Properties in the Ammonia Adsorbed Defective Graphene. Scientific Reports, 2016, 6, 33810.	1.6	3
17	Insertion of a naphthalenediimide unit in a metal-free donor–acceptor organic sensitizer for efficiency enhancement of a dye-sensitized solar cell. Dyes and Pigments, 2016, 134, 83-90.	2.0	21
18	A non-fullerene electron acceptor based on central carbazole and terminal diketopyrrolopyrrole functionalities for efficient, reproducible and solution-processable bulk-heterojunction devices. RSC Advances, 2016, 6, 28103-28109.	1.7	36

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19	Predicting a new phase (Tâ $\in$ <sup>2</sup> â $\in$ <sup>2</sup> ) of two-dimensional transition metal di-chalcogenides and strain-controlled topological phase transition. Nanoscale, 2016, 8, 4969-4975.	2.8	50
20	Single Layer Bismuth Iodide: Computational Exploration of Structural, Electrical, Mechanical and Optical Properties. Scientific Reports, 2015, 5, 17558.	1.6	67
21	An Electronâ€Accepting Chromophore Based on Fluorene and Naphthalenediimide Building Blocks for Solutionâ€Processable Bulk Heterojunction Devices. Asian Journal of Organic Chemistry, 2015, 4, 800-807.	1.3	11
22	Conjoint use of Dibenzosilole and Indanâ€1,3â€dione Functionalities to Prepare an Efficient Nonâ€Fullerene Acceptor for Solutionâ€Processable Bulkâ€Heterojunction Solar Cells. Asian Journal of Organic Chemistry, 2015, 4, 1096-1102.	1.3	23
23	Isoindigo-Based Small Molecules with Varied Donor Components for Solution-Processable Organic Field Effect Transistor Devices. Molecules, 2015, 20, 17362-17377.	1.7	8
24	Significant Improvement of Optoelectronic and Photovoltaic Properties by Incorporating Thiophene in a Solution-Processable D–A–D Modular Chromophore. Molecules, 2015, 20, 21787-21801.	1.7	10
25	Chemically Altering the Solubility and Durability of Dyes for Sensitized Solar Cells. Organic Letters, 2015, 17, 4022-4025.	2.4	14
26	Crowning of dibenzosilole with a naphthalenediimide functional group to prepare an electron acceptor for organic solar cells. Dyes and Pigments, 2015, 120, 314-321.	2.0	12
27	Optical properties of a conjugated-polymer-sensitised solar cell: the effect of interfacial structure. Physical Chemistry Chemical Physics, 2015, 17, 14489-14494.	1.3	0
28	Small molecules containing rigidified thiophenes and a cyanopyridone acceptor unit for solution-processable bulk-heterojunction solar cells. Dyes and Pigments, 2015, 119, 122-132.	2.0	21
29	Prediction of novel alloy phases of Al with Sc or Ta. Scientific Reports, 2015, 5, 9909.	1.6	23
30	Improvement of optoelectronic and photovoltaic properties through the insertion of a naphthalenediimide unit in donor–acceptor oligothiophenes. RSC Advances, 2015, 5, 4411-4415.	1.7	14
31	New organic sensitizers using 4-(cyanomethyl)benzoic acid as an acceptor group for dye-sensitized solar cell applications. Dyes and Pigments, 2015, 113, 280-288.	2.0	16
32	N-Alkyl- and N-aryl-dithieno[3,2-b:2′,3′-d]pyrrole-containing organic dyes for efficient dye-sensitized solar cells. Tetrahedron, 2014, 70, 2141-2150.	1.0	16
33	Novel organic sensitizer based on directly linked oligothiophenes to donor nitrogen atom for efficient dye-sensitized solar cells. Synthetic Metals, 2014, 193, 102-109.	2.1	4
34	Symmetrical and unsymmetrical donor–acceptor–donor organic dyes: Design, synthesis and characterization. Engineering panchromic absorbance. Dyes and Pigments, 2014, 108, 15-23.	2.0	5
35	Conformational transitions and dynamics of thermal responsive poly(N-isopropylacrylamide) polymers as revealed by molecular simulation. European Polymer Journal, 2014, 55, 153-159.	2.6	32
36	A diketopyrrolopyrrole and benzothiadiazole based small molecule electron acceptor: design, synthesis, characterization and photovoltaic properties. RSC Advances, 2014, 4, 57635-57638.	1.7	43

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37	A solution-processable electron acceptor based on diketopyrrolopyrrole and naphthalenediimide motifs for organic solar cells. Tetrahedron Letters, 2014, 55, 4430-4432.	0.7	35
38	A non-fullerene electron acceptor based on fluorene and diketopyrrolopyrrole building blocks for solution-processable organic solar cells with an impressive open-circuit voltage. Physical Chemistry Chemical Physics, 2014, 16, 23837-23842.	1.3	63
39	<i>N</i> Alkyl functionalized barbituric and thiobarbituric acid bithiophene derivatives for vacuum deposited n-channel OFETs. Journal of Materials Chemistry C, 2014, 2, 3895-3899.	2.7	15
40	Donor–Acceptor–Donor Modular Small Organic Molecules Based on the Naphthalene Diimide Acceptor Unit for Solution-Processable Photovoltaic Devices. Journal of Electronic Materials, 2014, 43, 3243-3254.	1.0	17
41	Aggregation of a Dibenzo[ <i>b</i> , <i>def</i> ]chrysene Based Organic Photovoltaic Material in Solution. Journal of Physical Chemistry B, 2014, 118, 6839-6849.	1.2	8
42	Tailoring highly conductive graphene nanoribbons from small polycyclic aromatic hydrocarbons: a computational study. Journal of Physics Condensed Matter, 2013, 25, 275301.	0.7	1
43	The impact of tetrahedral capping groups and device processing conditions on the crystal packing, thin film features and OFET hole mobility of 7,14-bis(ethynyl)dibenzo[b,def]chrysenes. Journal of Materials Chemistry C, 2013, 1, 6299.	2.7	17
44	Cyanomethylbenzoic Acid: An Acceptor for Donor–π–Acceptor Chromophores Used in Dye‣ensitized Solar Cells. ChemSusChem, 2013, 6, 256-260.	3.6	47
45	Indan-1,3-dione electron-acceptor small molecules for solution-processable solar cells: a structure–property correlation. Chemical Communications, 2013, 49, 6307.	2.2	106
46	Anomalous length dependence of the conductance of graphene nanoribbons with zigzag edges. Journal of Chemical Physics, 2013, 138, 014704.	1.2	2
47	Anomalous length dependence of conductance of aromatic nanoribbons with amine anchoring groups. Physical Review B, 2012, 86, .	1.1	4
48	Molecular engineering for panchromatic absorbing oligothiophene donor–π–acceptor organic semiconductors. Tetrahedron, 2012, 68, 9440-9447.	1.0	32
49	Absorption enhancement of oligothiophene dyes through the use of a cyanopyridone acceptor group in solution-processed organic solar cells. Chemical Communications, 2012, 48, 1889.	2.2	66
50	From fused aromatics to graphene-like nanoribbons: The effects of multiple terminal groups, length and symmetric pathways on charge transport. Physical Review B, 2011, 84, .	1.1	5
51	Photo-spectroscopic properties of benzothiadiazole-containing pendant polymers for photovoltaic applications. Journal of Photochemistry and Photobiology A: Chemistry, 2011, 220, 102-112.	2.0	5
52	Ground state structure of <mml:math <br="" xmlns:mml="http://www.w3.org/1998/Math/MathML">display="inline"&gt;<mml:mrow><mml:msub><mml:mrow><mml:mtext>BaZrO</mml:mtext></mml:mrow><mml:m A comparative first-principles study. Physical Review B, 2009, 79, .</mml:m </mml:msub></mml:mrow></mml:math>	117 <b>131</b> <td>l:r<b>ת א</b>&gt;</td>	l:r <b>ת א</b> >
53	Simulation of proton diffusion in In-doped CaZrO3. Solid State Ionics, 2008, 179, 871-874.	1.3	11

<sup>54</sup>Chemisorption of Molecular Hydrogen on Carbon Nanotubes: A Route to Effective Hydrogen Storage?.1.543Journal of Physical Chemistry C, 2008, 112, 12568-12575.1.543

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55	Proton Mobility in the In-Doped CaZrO3Perovskite Oxide. Chemistry of Materials, 2007, 19, 2842-2851.	3.2	27
56	Chemisorbed and Physisorbed Structures for 1,10-Phenanthroline and Dipyrido[3,2- <i>a</i> :2â€~,3â€~- <i>c</i> ]phenazine on Au(111). Journal of Physical Chemistry C, 2007, 111, 17285-17296.	1.5	25
57	The Green's Function Density Functional Tight-Binding (gDFTB) Method for Molecular Electronic Conductionâ€. Journal of Physical Chemistry A, 2007, 111, 5692-5702.	1.1	32
58	Adsorption of Benzene on Copper, Silver, and Gold Surfaces. Journal of Chemical Theory and Computation, 2006, 2, 1093-1105.	2.3	141
59	The Nature of the Adsorption of Nucleobases on the Gold [111] Surface. Journal of Physical Chemistry B, 2006, 110, 23467-23471.	1.2	114
60	FUNCTIONALIZATION OF SEMICONDUCTOR SURFACES BY ORGANIC LAYERS: CONCERTED CYCLOADDITION VERSUS STEPWISE FREE-RADICAL REACTION MECHANISMS. , 2006, , 333-360.		7
61	What Determines the Sticking Probability of Water Molecules on Ice?. Physical Review Letters, 2005, 95, 223201.	2.9	48
62	Coexistence of Multiple Conformations in Cysteamine Monolayers on Au(111). Journal of Physical Chemistry B, 2005, 109, 15355-15367.	1.2	79
63	The structure, energetics, and nature of the chemical bonding of phenylthiol adsorbed on the Au(111) surface: Implications for density-functional calculations of molecular-electronic conduction. Journal of Chemical Physics, 2005, 122, 094708.	1.2	150
64	DISSOCIATED WATER ON Si(100): RELATION BETWEEN STM TOPOGRAPH AND ACTUAL GEOMETRY. Surface Review and Letters, 2004, 11, 185-190.	0.5	3
65	Molecular Electronics: From Basic Chemical Principles to Photosynthesis to Steady-State Through-Molecule Conductivity to Computer Architectures. Australian Journal of Chemistry, 2004, 57, 1133.	0.5	14
66	Adsorption sites of maleic anhydride on Si(100) revisited: inter- versus intra-row attachment. Chemical Physics Letters, 2004, 385, 341-344.	1.2	5
67	The Appropriateness of Density-Functional Theory for the Calculation of Molecular Electronics Properties. Annals of the New York Academy of Sciences, 2003, 1006, 235-251.	1.8	107
68	Modeling the adsorption of norbornadiene on the Si(001) surface: The predominance of non-[2+2]-cycloaddition products. Journal of Chemical Physics, 2003, 119, 1115-1126.	1.2	12
69	Adsorption of Pyridine on the Gold(111) Surface:  Implications for "Alligator Clips―for Molecular Wires. Journal of Physical Chemistry B, 2002, 106, 6740-6747.	1.2	113
70	Adsorption of ammonia on the gold (111) surface. Journal of Chemical Physics, 2002, 116, 8981-8987.	1.2	112
71	Embedded atom method study of surface-confined Al on Ni(001). Surface Science, 1999, 442, 256-264.	0.8	9
72	Multiphonon He atom scattering from Xe overlayers on Cu(111) and Cu(001) surfaces. Journal of Chemical Physics, 1997, 106, 9922-9929.	1.2	16

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73	Multiphonon atom-surface scattering in the collision system He → Cu(001). Surface Science, 1997, 370, 47-54.	0.8	12
74	Reinvestigation of the surface reconstruction of Cu(001)-(2 × 2)p4g-Pd. Surface Science, 1997, 394, L131-L137.	0.8	22
75	Energy dissipation of fast neutral beams scattered at glancing angles from crystal surfaces. Surface Science, 1996, 368, 71-75.	0.8	5
76	Multiphonon He atom scattering in collisions. Surface Science, 1996, 368, 232-238.	0.8	7
77	Quantum versus semiclassical treatment of multiphonon effects in He-atom scattering from surfaces. Physical Review B, 1995, 52, 12307-12328.	1.1	35