Erin Johnson

List of Publications by Year
in descending order

139 papers	22,628 citations	50276 46 h-index	10734 138 g-index
152 all docs	152 docs citations	152 times ranked	18069 citing authors

#	Article	IF	Citations
1	Delocalization error: The greatest outstanding challenge in densityâ€functional theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2023, 13, .	14.6	43
2	Identification of a Nitrenoid Reductive Elimination Pathway in Nickel-Catalyzed Câ€“N Cross-Coupling. ACS Catalysis, 2022, 12, 1475-1480.	11.2	10
3	A density-functional benchmark of vibrational free-energy corrections for molecular crystal polymorphism. Journal of Chemical Physics, 2022, 156, 114108.	3.0	7
4	The Relative Thermodynamic Stability of Diamond and Graphite. Angewandte Chemie, 2021, 133, 1570-1573.	2.0	0
5	Improved quantitative crystal-structure comparison using powder diffractograms via anisotropic volume correction. CrystEngComm, 2021, 23, 7118-7131.	2.6	4
6	Theoretical investigation of polymorph- and coformer-dependent photoluminescence in molecular crystals. CrystEngComm, 2021, 23, 4264-4271.	2.6	9
7	Theoretical modeling of structural superlubricity in rotated bilayer graphene, hexagonal boron nitride, molybdenum disulfide, and blue phosphorene. Nanoscale, 2021, 13, 14399-14407.	5.6	13
8	Directed Ortho and Remote Metalation of Naphthalene 1,8-Diamide: Complementing S_EAr Reactivity for the Synthesis of Substituted Naphthalenes. Organic Letters, 2021, 23, 1966-1973.	4.6	2
9	Interplay between London Dispersion, Hubbard U, and Metastable States for Uranium Compounds. Journal of Physical Chemistry A, 2021, 125, 2791-2799.	2.5	4
10	Improved Charge Transfer and Barrier Lowering across a Auâ€“MoS₂ Interface through Insertion of a Layered Ca₂N Electride. Journal of Physical Chemistry C, 2021, 125, 11656-11664.	3.1	5
11	Requirements for an accurate dispersion-corrected density functional. Journal of Chemical Physics, 2021, 154, 230902.	3.0	39
12	Computational Screening of Chiral Organic Semiconductors: Exploring Side-Group Functionalization and Assembly to Optimize Charge Transport. Crystal Growth and Design, 2021, 21, 5036-5049.	3.0	11
13	The Relative Thermodynamic Stability of Diamond and Graphite. Angewandte Chemie - International Edition, 2021, 60, 1546-1549.	13.8	8
14	Quantum Chemical Methods for Modeling Covalent Modification of Biological Thiols. Journal of Computational Chemistry, 2020, 41, 427-438.	3.3	31
15	Analysis of Density-Functional Errors for Noncovalent Interactions between Charged Molecules. Journal of Physical Chemistry A, 2020, 124, 353-361.	2.5	5
16	Theoretical investigation of amino-acid adsorption on hydroxylated quartz surfaces: dispersion can determine enantioselectivity. Physical Chemistry Chemical Physics, 2020, 22, 16571-16578.	2.8	7
17	Application of XDM to ionic solids: The importance of dispersion for bulk moduli and crystal geometries. Journal of Chemical Physics, 2020, 153, 054121.	3.0	11
18	Hydrostibination of Alkynes: A Radical Mechanism**. Chemistry - A European Journal, 2020, 26, 17134-17142.	3.3	8

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19	Potent Inhibition of Mandelate Racemase by Boronic Acids: Boron as a Mimic of a Carbon Acid Center. Biochemistry, 2020, 59, 3026-3037.	2.5	6
20	Asymptotic Pairwise Dispersion Corrections Can Describe Layered Materials Accurately. Journal of Physical Chemistry Letters, 2020, 11, 2298-2302.	4.6	17
21	Computational modeling of piezochromism in molecular crystals. Journal of Chemical Physics, 2020, 152, 234106.	3.0	4
22	What is â€œmany-bodyâ€•dispersion and should I worry about it?. Physical Chemistry Chemical Physics, 2020, 22, 8266-8276.	2.8	30
23	Dispersion XDM with Hybrid Functionals: Delocalization Error and Halogen Bonding in Molecular Crystals. Journal of Chemical Theory and Computation, 2019, 15, 4933-4944.	5.3	22
24	Clusters in Liquid Fatty Acids: Structure and Role in Nucleation. Journal of Physical Chemistry B, 2019, 123, 7043-7054.	2.6	8
25	Origin of Nanoscale Friction Contrast between Supported Graphene, MoS₂, and a Graphene/MoS₂ Heterostructure. Nano Letters, 2019, 19, 5496-5505.	9.1	115
26	Crystal-energy landscapes of active pharmaceutical ingredients using composite approaches. CrystEngComm, 2019, 21, 5995-6009.	2.6	14
27	Gold(<scp>i</scp>) sulfide: unusual bonding and an unexpected computational challenge in a simple solid. Chemical Science, 2019, 10, 6467-6475.	7.4	12
28	Composite and Low-Cost Approaches for Molecular Crystal Structure Prediction. Journal of Chemical Theory and Computation, 2018, 14, 2265-2276.	5.3	18
29	Structure and formation of highly luminescent protein-stabilized gold clusters. Chemical Science, 2018, 9, 2782-2790.	7.4	76
30	A computational exploration of the crystal energy and charge-carrier mobility landscapes of the chiral [6]helicene molecule. Nanoscale, 2018, 10, 1865-1876.	5.6	48
31	Application of Diazaphospholidine/Diazaphospholene-Based Bisphosphines in Room-Temperature Nickel-Catalyzed C(sp²)â€“N Cross-Couplings of Primary Alkylamines with (Hetero)aryl Chlorides and Bromides. ACS Catalysis, 2018, 8, 5328-5339.	11.2	26
32	Effect of a Metal Substrate on Interlayer Interactions in Bilayer Graphene. Journal of Physical Chemistry C, 2018, 122, 8910-8918.	3.1	9
33	Density-functional description of alkalides: introducing the alkalide state. Physical Chemistry Chemical Physics, 2018, 20, 26710-26718.	2.8	9
34	Are dispersion corrections accurate outside equilibrium? A case study on benzene. Beilstein Journal of Organic Chemistry, 2018, 14, 1181-1191.	2.2	15
35	Communication: Beckeâ€™s virial exciton model gives accurate charge-transfer excitation energies. Journal of Chemical Physics, 2018, 149, 231101.	3.0	9
36	Pervasive Delocalisation Error Causes Spurious Proton Transfer in Organic Acidâ€“Base Coâ€Crystals. Angewandte Chemie, 2018, 130, 15122-15126.	2.0	10

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37	Pervasive Delocalisation Error Causes Spurious Proton Transfer in Organic Acidâ€“Base Coâ€Crystals. Angewandte Chemie - International Edition, 2018, 57, 14906-14910.	13.8	45
38	Probing the Influence of PAd-DalPhos Ancillary Ligand Structure on Nickel-Catalyzed Ammonia Cross-Coupling. Organometallics, 2018, 37, 4015-4023.	2.3	10
39	Non-Covalent Interactions in Molecular Crystals: Exploring the Accuracy of the Exchange-Hole Dipole Moment Model with Local Orbitals. Journal of Chemical Theory and Computation, 2018, 14, 5715-5724.	5.3	9
40	Theoretical Descriptors of Electrides. Journal of Physical Chemistry A, 2018, 122, 9371-9391.	2.5	63
41	Pressure-Induced Isostructural Antiferromagneticâ€“Ferromagnetic Transition in an Organic Electride. Journal of Physical Chemistry C, 2018, 122, 12742-12747.	3.1	14
42	Quantitative Electron Delocalization in Solids from Maximally Localized Wannier Functions. Journal of Chemical Theory and Computation, 2018, 14, 4699-4710.	5.3	12
43	Communication: Correct charge transfer in CT complexes from the Beckeâ€™05 density functional. Journal of Chemical Physics, 2018, 148, 211101.	3.0	20
44	Evaluating the London Dispersion Coefficients of Protein Force Fields Using the Exchange-Hole Dipole Moment Model. Journal of Physical Chemistry B, 2018, 122, 6690-6701.	2.6	32
45	The effect of electronic excitation on London dispersion. Canadian Journal of Chemistry, 2018, 96, 730-737.	1.1	9
46	Thermodynamic cycles of the alkali metalâ€“ligand complexes central to electride formation. Physical Chemistry Chemical Physics, 2017, 19, 12816-12825.	2.8	7
47	Adsorption of graphene to nickel (111) using the exchange-hole dipole moment model. Carbon, 2017, 118, 184-191.	10.3	18
48	Exchange-Hole Dipole Dispersion Model for Accurate Energy Ranking in Molecular Crystal Structure Prediction. Journal of Chemical Theory and Computation, 2017, 13, 441-450.	5.3	56
49	The ionic versus metallic nature of 2D electrides: a density-functional description. Physical Chemistry Chemical Physics, 2017, 19, 27343-27352.	2.8	16
50	Exchange-Hole Dipole Dispersion Model for Accurate Energy Ranking in Molecular Crystal Structure Prediction II: Nonplanar Molecules. Journal of Chemical Theory and Computation, 2017, 13, 5332-5342.	5.3	31
51	Hydroboration Catalyzed by 1,2,4,3-Triazaphospholenes. Organic Letters, 2017, 19, 5565-5568.	4.6	44
52	Interrogating the Beckeâ€™05 density functional for non-locality information. Journal of Chemical Physics, 2017, 147, 154103.	3.0	15
53	Adsorption of graphene to metal (111) surfaces using the exchange-hole dipole moment model. Carbon, 2017, 124, 531-540.	10.3	22
54	Bisphosphineâ€Ligated Nickel Preâ€catalysts in C(sp²)â€“N Crossâ€Couplings of Aryl Chlorides: A Comparison of Nickel(I) and Nickel(II). Advanced Synthesis and Catalysis, 2017, 359, 2972-2980.	4.3	51

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55	Emergent Properties of an Organic Semiconductor Driven by its Molecular Chirality. ACS Nano, 2017, 11, 8329-8338.	14.6	136
56	Evaluating Force-Field London Dispersion Coefficients Using the Exchange-Hole Dipole Moment Model. Journal of Chemical Theory and Computation, 2017, 13, 6146-6157.	5.3	40
57	Communication: DFT treatment of strong correlation in 3d transition-metal diatomics. Journal of Chemical Physics, 2017, 146, 211105.	3.0	42
58	The Exchange-Hole Dipole Moment Dispersion Model. , 2017, , 169-194.		37
59	Reevaluating the Stability and Prevalence of Conglomerates: Implications for Preferential Crystallization. Crystal Growth and Design, 2016, 16, 6055-6059.	3.0	29
60	The explicit examination of the magnetic states of electrides. Physical Chemistry Chemical Physics, 2016, 18, 27326-27335.	2.8	16
61	Evaluation of Shear-Slip Transitions in Crystalline Aspirin by Density-Functional Theory. Crystal Growth and Design, 2016, 16, 6867-6873.	3.0	17
62	van der Waals potential energy surfaces from the exchange-hole dipole moment dispersion model. Canadian Journal of Chemistry, 2016, 94, 1049-1056.	1.1	1
63	Exchangeâ€“Correlation Effects for Noncovalent Interactions in Density Functional Theory. Journal of Chemical Theory and Computation, 2016, 12, 3160-3175.	5.3	24
64	Surface Adsorption from the Exchange-Hole Dipole Moment Dispersion Model. Journal of Chemical Theory and Computation, 2016, 12, 3305-3315.	5.3	43
65	Counterintuitive electron localisation from density-functional theory with polarisable solvent models. Journal of Chemical Physics, 2015, 143, 184112.	3.0	11
66	Chemical bonding and surface interactions in Bi2Se3 and Bi4Se3. Computational and Theoretical Chemistry, 2015, 1053, 238-244.	2.5	14
67	New XDM-corrected potential energy surfaces for Arâ€“NO(X2Î): A comparison with CCSD(T) calculations and experiments. Journal of Chemical Physics, 2015, 142, 024302.	3.0	6
68	(Ag,Cu)â€“Taâ€“O Ternaries As High-Temperature Solid-Lubricant Coatings. ACS Applied Materials & Interfaces, 2015, 7, 15422-15429.	8.0	32
69	Balancing Exchange Mixing in Density-Functional Approximations for Iron Porphyrin. Journal of Chemical Theory and Computation, 2015, 11, 3022-3028.	5.3	22
70	Kinetics of the Addition of Olefins to Si-Centered Radicals: The Critical Role of Dispersion Interactions Revealed by Theory and Experiment. Journal of Physical Chemistry A, 2015, 119, 5883-5888.	2.5	5
71	Oscillatory motion in layered materials: graphene, boron nitride, and molybdenum disulfide. Nanotechnology, 2015, 26, 165701.	2.6	18
72	Predicting Energetics of Supramolecular Systems Using the XDM Dispersion Model. Journal of Chemical Theory and Computation, 2015, 11, 4033-4040.	5.3	39

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73	Density-functional errors in ionization potential with increasing system size. Journal of Chemical Physics, 2015, 142, 184106.	3.0	52
74	Judging Density-Functional Approximations: Some Pitfalls of Statistics. Topics in Current Chemistry, 2014, , 81-95.	4.0	10
75	Local-hybrid functional based on the correlation length. Journal of Chemical Physics, 2014, 141, 124120.	3.0	38
76	Halogen Bonding from Dispersion-Corrected Density-Functional Theory: The Role of Delocalization Error. Journal of Chemical Theory and Computation, 2014, 10, 5436-5447.	5.3	100
77	Critic2: A program for real-space analysis of quantum chemical interactions in solids. Computer Physics Communications, 2014, 185, 1007-1018.	7.5	497
78	Metallophilic interactions from dispersion-corrected density-functional theory. Journal of Chemical Physics, 2014, 140, 18A504.	3.0	47
79	Density-functional description of electrides. Physical Chemistry Chemical Physics, 2014, 16, 14584-14593.	2.8	76
80	The role of roughness-induced damping in the oscillatory motion of bilayer graphene. Nanotechnology, 2014, 25, 425703.	2.6	2
81	Chemical Basis of the Tribological Properties of AgTaO₃ Crystal Surfaces. Journal of Physical Chemistry C, 2014, 118, 17577-17584.	3.1	18
82	Predicting the Relative Solubilities of Racemic and Enantiopure Crystals by Densityâ€Functional Theory. Angewandte Chemie - International Edition, 2014, 53, 7879-7882.	13.8	56
83	Many-body dispersion interactions from the exchange-hole dipole moment model. Journal of Chemical Physics, 2013, 138, 054103.	3.0	65
84	Performance of conventional and dispersion-corrected density-functional theory methods for hydrogen bonding interaction energies. Physical Chemistry Chemical Physics, 2013, 15, 12821.	2.8	120
85	A density functional for strong correlation in atoms. Journal of Chemical Physics, 2013, 139, 074110.	3.0	15
86	Carbon Nanotube Chirality Determines Efficiency of Electron Transfer to Fullerene in All-Carbon Photovoltaics. Journal of Physical Chemistry Letters, 2013, 4, 2914-2918.	4.6	46
87	Effect of tip shape on atomic-friction at graphite step edges. Applied Physics Letters, 2013, 103, 081601.	3.3	30
88	An empirical model for silver tantalate. Modelling and Simulation in Materials Science and Engineering, 2013, 21, 055002.	2.0	12
89	Large negative thermal expansion of a polymer driven by a submolecular conformational change. Nature Chemistry, 2013, 5, 1035-1041.	13.6	103
90	Modeling Noncovalent Radicalâ€“Molecule Interactions Using Conventional Density-Functional Theory: Beware Erroneous Charge Transfer. Journal of Physical Chemistry A, 2013, 117, 947-952.	2.5	41

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91	Non-covalent interactions and thermochemistry using XDM-corrected hybrid and range-separated hybrid density functionals. Journal of Chemical Physics, 2013, 138, 204109.	3.0	130
92	Extreme density-driven delocalization error for a model solvated-electron system. Journal of Chemical Physics, 2013, 139, 184116.	3.0	93
93	Contributions of pauli repulsions to the energetics and physical properties computed in QM/MM methods. Journal of Computational Chemistry, 2013, 34, 2380-2388.	3.3	9
94	Efficient basis sets for non-covalent interactions in XDM-corrected density-functional theory. Journal of Chemical Physics, 2013, 139, 214109.	3.0	29
95	Delocalization error of density-functional approximations: A distinct manifestation in hydrogen molecular chains. Journal of Chemical Physics, 2012, 137, 214106.	3.0	66
96	Revealing non-covalent interactions in solids: NCI plots revisited. Physical Chemistry Chemical Physics, 2012, 14, 12165.	2.8	279
97	Adsorption of Organic Molecules on Kaolinite from the Exchange-Hole Dipole Moment Dispersion Model. Journal of Chemical Theory and Computation, 2012, 8, 5124-5131.	5.3	50
98	Variational fractional-spin density-functional theory for diradicals. Journal of Chemical Physics, 2012, 137, 114112.	3.0	27
99	A benchmark for non-covalent interactions in solids. Journal of Chemical Physics, 2012, 137, 054103.	3.0	300
100	Density-Functional Errors in Alkanes: A Real-Space Perspective. Journal of Chemical Theory and Computation, 2012, 8, 2676-2681.	5.3	16
101	Van der Waals interactions in solids using the exchange-hole dipole moment model. Journal of Chemical Physics, 2012, 136, 174109.	3.0	197
102	Analysis of Hydrogen-Bond Interaction Potentials from the Electron Density: Integration of Noncovalent Interaction Regions. Journal of Physical Chemistry A, 2011, 115, 12983-12990.	2.5	339
103	Singletâ^'Triplet Energy Gaps for Diradicals from Fractional-Spin Density-Functional Theory. Journal of Physical Chemistry A, 2011, 115, 76-83.	2.5	107
104	NCIPLOT: A Program for Plotting Noncovalent Interaction Regions. Journal of Chemical Theory and Computation, 2011, 7, 625-632.	5.3	2,897
105	Dependence of dispersion coefficients on atomic environment. Journal of Chemical Physics, 2011, 135, 234109.	3.0	31
106	Communication: A density functional with accurate fractional-charge and fractional-spin behaviour for s-electrons. Journal of Chemical Physics, 2011, 135, 081103.	3.0	31
107	Revealing Noncovalent Interactions. Journal of the American Chemical Society, 2010, 132, 6498-6506.	13.7	6,465
108	Spin-state splittings, highest-occupied-molecular-orbital and lowest-unoccupied-molecular-orbital energies, and chemical hardness. Journal of Chemical Physics, 2010, 133, 164107.	3.0	14

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109	Oscillations in meta-generalized-gradient approximation potential energy surfaces for dispersion-bound complexes. Journal of Chemical Physics, 2009, 131, 034111.	3.0	153
110	Convergence of calculated nuclear magnetic resonance chemical shifts in a protein with respect to quantum mechanical model size. Computational and Theoretical Chemistry, 2009, 898, 56-61.	1.5	16
111	Radicals as hydrogen bond donors and acceptors. Interdisciplinary Sciences, Computational Life Sciences, 2009, 1, 133-140.	3.6	15
112	Dispersion interactions in densityâ€functional theory. Journal of Physical Organic Chemistry, 2009, 22, 1127-1135.	1.9	322
113	Theoretical Study of Dispersion Binding of Hydrocarbon Molecules to Hydrogen-Terminated Silicon(100)-2Ã—1. Journal of Physical Chemistry C, 2009, 113, 5681-5689.	3.1	24
114	Pentacene Binds Strongly to Hydrogen-Terminated Silicon Surfaces Via Dispersion Interactions. Journal of Physical Chemistry C, 2009, 113, 9969-9973.	3.1	12
115	Tests of an exact-exchange-based density-functional theory on transition-metal complexes. Canadian Journal of Chemistry, 2009, 87, 1369-1373.	1.1	24
116	A unified density-functional treatment of dynamical, nondynamical, and dispersion correlations. II. Thermochemical and kinetic benchmarks. Journal of Chemical Physics, 2008, 128, 124105.	3.0	39
117	Delocalization errors in density functionals and implications for main-group thermochemistry. Journal of Chemical Physics, 2008, 129, 204112.	3.0	159
118	Density functionals and transition-metal atoms. Journal of Chemical Physics, 2007, 126, 184104.	3.0	29
119	Exchange-hole dipole moment and the dispersion interaction revisited. Journal of Chemical Physics, 2007, 127, 154108.	3.0	432
120	A unified density-functional treatment of dynamical, nondynamical, and dispersion correlations. Journal of Chemical Physics, 2007, 127, 124108.	3.0	193
121	Lone Pairâ^Ï€ and Ï€â^Ï€ Interactions Play an Important Role in Proton-Coupled Electron Transfer Reactions. Journal of the American Chemical Society, 2007, 129, 6199-6203.	13.7	185
122	Hydrogen-bond strengths in large complexes: Efficient calculations using locally dense basis sets. Chemical Physics Letters, 2007, 435, 201-207.	2.6	12
123	A post-Hartree-Fock model of intermolecular interactions: Inclusion of higher-order corrections. Journal of Chemical Physics, 2006, 124, 174104.	3.0	896
124	Exchange-hole dipole moment and the dispersion interaction: High-order dispersion coefficients. Journal of Chemical Physics, 2006, 124, 014104.	3.0	184
125	A simple effective potential for exchange. Journal of Chemical Physics, 2006, 124, 221101.	3.0	1,200
126	Structure and binding energies in van der Waals dimers: Comparison between density functional theory and correlated ab initio methods. Chemical Physics Letters, 2006, 419, 333-339.	2.6	136

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127	Van der Waals interactions from the exchange hole dipole moment: Application to bio-organic benchmark systems. Chemical Physics Letters, 2006, 432, 600-603.	2.6	61
128	Reply to comment on â€˜Application of 25 density functionals to dispersion-bound homomolecular dimersâ€™ [Chem. Phys. Lett. 394 (2004) 334â€“338]. Chemical Physics Letters, 2005, 401, 595-596.	2.6	10
129	Efficient silicon surface and cluster modeling using quantum capping potentials. Journal of Chemical Physics, 2005, 122, 044708.	3.0	42
130	Exchange-hole dipole moment and the dispersion interaction. Journal of Chemical Physics, 2005, 122, 154104.	3.0	497
131	A density-functional model of the dispersion interaction. Journal of Chemical Physics, 2005, 123, 154101.	3.0	1,150
132	A post-Hartreeâ€“Fock model of intermolecular interactions. Journal of Chemical Physics, 2005, 123, 024101.	3.0	735
133	Density Functional Theory Based Model Calculations for Accurate Bond Dissociation Enthalpies. Part 3. A Single Approach for Xâ€”H, Xâ€”X, and Xâ€”Y, (X, Y: C, N, O, S, Halogen) Bonds.. ChemInform, 2004, 35, no.	0.0	0
134	Application of 25 density functionals to dispersion-bound homomolecular dimers. Chemical Physics Letters, 2004, 394, 334-338.	2.6	237
135	Density Functional Theory Based Model Calculations for Accurate Bond Dissociation Enthalpies. 3. A Single Approach for Xâˆ’H, Xâˆ’X, and Xâˆ’Y (X, Y = C, N, O, S, Halogen) Bonds. Journal of Physical Chemistry A, 2003, 107, 9953-9963.	2.5	109
136	Patterning of Vinylferrocene on Hâˆ’Si(100) via Self-Directed Growth of Molecular Lines and STM-Induced Decomposition. Nano Letters, 2002, 2, 807-810.	9.1	139
137	Naphthalene Diols:Â A New Class of Antioxidants Intramolecular Hydrogen Bonding in Catechols, Naphthalene Diols, and Their Aryloxyl Radicals. Journal of Organic Chemistry, 2002, 67, 5190-5196.	3.2	154
138	Predicting the Activity of Phenolic Antioxidants:Â Theoretical Method, Analysis of Substituent Effects, and Application to Major Families of Antioxidants. Journal of the American Chemical Society, 2001, 123, 1173-1183.	13.7	1,367
139	Noncovalent Interactions in Organic Radicals: Pancake, Ïƒ-Hole, and H-Bonding in F2HbimDTDA. Crystal Growth and Design, 0, , .	3.0	2