Blint Aradi

List of Publications by Citations

68 papers	3,562 citations	26 h-index	59 g-index
70 ext. papers	4,162 ext. citations	4.4 avg, IF	5.44 L-index

#	Paper	IF	Citations
68	DFTB+, a sparse matrix-based implementation of the DFTB method. *Journal of Physical Chemistry A*, **2007**, 111, 5678-84	2.8	1327
67	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. *Journal of Chemical Physics*, **2020**, 152, 124101	3.9	210
66	An Improved Self-Consistent-Charge Density-Functional Tight-Binding (SCC-DFTB) Set of Parameters for Simulation of Bulk and Molecular Systems Involving Titanium. *Journal of Chemical Theory and Computation*, **2010**, 6, 266-78	6.4	155
65	Band Lineup and Charge Carrier Separation in Mixed Rutile-Anatase Systems. *Journal of Physical Chemistry C*, **2011**, 115, 3443-3446	3.8	147
64	Choosing the correct hybrid for defect calculations: A case study on intrinsic carrier trapping in Ga2O3. *Physical Review B*, **2017**, 95,	3.3	144
63	Formation of NV centers in diamond: A theoretical study based on calculated transitions and migration of nitrogen and vacancy related defects. *Physical Review B*, **2014**, 89,	3.3	113
62	Toward an Accurate Density-Functional Tight-Binding Description of Zinc-Containing Compounds. *Journal of Chemical Theory and Computation*, **2009**, 5, 605-14	6.4	100
61	Proper surface termination for luminescent near-surface NV centers in diamond. *Nano Letters*, **2014** , 14, 4772-7	11.5	92
60	Nonadiabatic Molecular Dynamics for Thousand Atom Systems: A Tight-Binding Approach toward PYXAID. *Journal of Chemical Theory and Computation*, **2016**, 12, 1436-48	6.4	82
59	The self-consistent charge density functional tight binding method applied to liquid water and the hydrated excess proton: benchmark simulations. *Journal of Physical Chemistry B*, **2010**, 114, 6922-31	3.4	63
58	SCC-DFTB parameters for simulating hybrid gold-thiolates compounds. *Journal of Computational Chemistry*, **2015**, 36, 2075-87	3.5	58
57	Theoretical study of the chemical gap tuning in silicon nanowires. *Physical Review B*, **2007**, 76,	3.3	58
56	Implementation and benchmark of a long-range corrected functional in the density functional based tight-binding method. *Journal of Chemical Physics*, **2015**, 143, 184107	3.9	53
55	Extensions of the Time-Dependent Density Functional Based Tight-Binding Approach. *Journal of Chemical Theory and Computation*, **2013**, 9, 4901-14	6.4	51
54	Water splitting and the band edge positions of TiO2. *Electrochimica Acta*, **2016**, 199, 27-34	6.7	48
53	Self-interaction and strong correlation in DFTB. *Journal of Physical Chemistry A*, **2007**, 111, 5671-7	2.8	47
52	Time-Dependent Extension of the Long-Range Corrected Density Functional Based Tight-Binding Method. *Journal of Chemical Theory and Computation*, **2017**, 13, 1737-1747	6.4	46

51	Parametrization of the SCC-DFTB Method for Halogens. *Journal of Chemical Theory and Computation*, **2013**, 9, 2939-49	6.4	45
50	Resolving the Controversy about the Band Alignment between Rutile and Anatase: The Role of OH⁄H+ Adsorption. *Journal of Physical Chemistry C*, **2015**, 119, 21952-21958	3.8	42
49	Accurate single-particle determination of the band gap in silicon nanowires. *Physical Review B*, **2007**, 76,	3.3	39
48	Accurate gap levels and their role in the reliability of other calculated defect properties. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 790-798	1.3	38
47	Graphene nucleation on a surface-molten copper catalyst: quantum chemical molecular dynamics simulations. *Chemical Science*, **2014**, 5, 3493-3500	9.4	36
46	Overcoordinated hydrogens in the carbon vacancy: donor centers of SiC. *Physical Review Letters*, **2000**, 84, 4926-9	7.4	34
45	Automated Repulsive Parametrization for the DFTB Method. *Journal of Chemical Theory and Computation*, **2011**, 7, 2654-64	6.4	27
44	Donor levels in Si nanowires determined by hybrid-functional calculations. *Physical Review B*, **2009**, 79,	3.3	27
43	Possible improvements to the self-consistent-charges density-functional tight-binding method within the second order. *Physica Status Solidi (B): Basic Research*, **2012**, 249, 259-269	1.3	25
42	Impurity-controlled dopant activation: Hydrogen-determined site selection of boron in silicon carbide. *Applied Physics Letters*, **2001**, 79, 2746-2748	3.4	25
41	Development of a Multicenter Density Functional Tight Binding Model for Plutonium Surface Hydriding. *Journal of Chemical Theory and Computation*, **2018**, 14, 2652-2660	6.4	21
40	Plasmon-driven sub-picosecond breathing of metal nanoparticles. *Nanoscale*, **2017**, 9, 12391-12397	7.7	20
39	Theoretical study of charge separation at the rutile□natase interface. *Physica Status Solidi - Rapid Research Letters*, **2014**, 8, 566-570	2.5	20
38	Extended Lagrangian Density Functional Tight-Binding Molecular Dynamics for Molecules and Solids. *Journal of Chemical Theory and Computation*, **2015**, 11, 3357-63	6.4	19
37	Anharmonicity of the C□H stretch mode in SiC: Unambiguous identification of hydrogen□silicon vacancy defect. *Applied Physics Letters*, **2002**, 80, 237-239	3.4	19
36	Self-Consistent-Charge Density-Functional Tight-Binding (SCC-DFTB) Parameters for Ceria in 0D to 3D. *Journal of Physical Chemistry C*, **2017**, 121, 4593-4607	3.8	18
35	Atomic Level Modeling of Extremely Thin Silicon-on-Insulator MOSFETs Including the Silicon Dioxide: Electronic Structure. *IEEE Transactions on Electron Devices*, **2015**, 62, 696-704	2.9	17
34	Role of Symmetry in the Stability and Electronic Structure of Titanium Dioxide Nanowires. *Journal of Physical Chemistry C*, **2011**, 115, 18494-18499	3.8	17

33	Native Defects in ZnO Nanowires: Atomic Relaxations, Relative Stability, and Defect Healing with Organic Acids. *Journal of Physical Chemistry C*, **2010**, 114, 18860-18865	3.8	17
32	Fully Atomistic Real-Time Simulations of Transient Absorption Spectroscopy. *Journal of Physical Chemistry Letters*, **2018**, 9, 4355-4359	6.4	14
31	Atomistic Modeling of Gate-All-Around Si-Nanowire Field-Effect Transistors. *IEEE Transactions on Electron Devices*, **2007**, 54, 3159-3167	2.9	14
30	Self-Consistent Potential Correction for Charged Periodic Systems. *Physical Review Letters*, **2021**, 126, 076401	7.4	14
29	Efficient Automatized Density-Functional Tight-Binding Parametrizations: Application to Group IV Elements. *Journal of Chemical Theory and Computation*, **2018**, 14, 2947-2954	6.4	13
28	Density-functional tight-binding for phosphine-stabilized nanoscale gold clusters. *Chemical Science*, **2020**, 11, 13113-13128	9.4	13
27	Density functional tight binding-based free energy simulations in the DFTB+ program. *Journal of Computational Chemistry*, **2018**, 39, 2452-2458	3.5	13
26	Optimized hybrid functionals for defect calculations in semiconductors. *Journal of Applied Physics*, **2019**, 126, 130901	2.5	12
25	Some like it shallower: p-type doping in SiC. *Physica Status Solidi (B): Basic Research*, **2003**, 235, 139-145	1.3	12
24	Permittivity of Oxidized Ultra-Thin Silicon Films From Atomistic Simulations. *IEEE Electron Device Letters*, **2015**, 36, 1076-1078	4.4	11
23	A Real-Time Time-Dependent Density Functional Tight-Binding Implementation for Semiclassical Excited State Electron-Nuclear Dynamics and Pump-Probe Spectroscopy Simulations. *Journal of Chemical Theory and Computation*, **2020**, 16, 4454-4469	6.4	11
22	Automatized Parameterization of the Density-functional Tight-binding Method. II. Two-center Integrals. *Journal of the Chinese Chemical Society*, **2016**, 63, 57-68	1.5	11
21	Possibility of a field effect transistor based on Dirac particles in semiconducting anatase-TiO2 nanowires. *Nano Letters*, **2013**, 13, 1073-9	11.5	10
20	Boron and aluminium doping in SiC and its passivation by hydrogen. *Journal of Physics Condensed Matter*, **2001**, 13, 9019-9026	1.8	10
19	The basic matrix library (BML) for quantum chemistry. *Journal of Supercomputing*, **2018**, 74, 6201-6219	2.5	8
18	How small nanodiamonds can be? MD study of the stability against graphitization. *Diamond and Related Materials*, **2013**, 33, 78-84	3.5	8
17	Ewald summation on a helix: A route to self-consistent charge density-functional based tight-binding objective molecular dynamics. *Journal of Chemical Physics*, **2013**, 139, 094110	3.9	8
16	Defect calculations with hybrid functionals in layered compounds and in slab models. *Physical Review B*, **2019**, 100,	3.3	8

15	SLABCC: Total energy correction code for charged periodic slab models. *Computer Physics Communications*, **2019**, 240, 101-105	4.2	7
14	Simulation of Impulsive Vibrational Spectroscopy. *Journal of Physical Chemistry A*, **2019**, 123, 2065-2072	2.8	6
13	Semi-Automated Creation of Density Functional Tight Binding Models through Leveraging Chebyshev Polynomial-Based Force Fields. *Journal of Chemical Theory and Computation*, **2021**, 17, 4435-4448	6.4	5
12	Curvature Constrained Splines for DFTB Repulsive Potential Parametrization. *Journal of Chemical Theory and Computation*, **2021**, 17, 1771-1781	6.4	5
11	Towards a simplified description of thermoelectric materials: accuracy of approximate density functional theory for phonon dispersions. *Journal of Physics Condensed Matter*, **2019**, 31, 395901	1.8	4
10	Towards atomic level simulation of electron devices including the semiconductor-oxide interface **2014**,		4
9	Water Reactions on Reconstructed Rutile TiO2: A Density Functional Theory/Density Functional Tight Binding Approach. *Journal of Physical Chemistry C*, **2021**, 125, 13234-13246	3.8	4
8	Super-cell calculation of the nitrogen defect in diamond and cubic silicon carbide. *Diamond and Related Materials*, **2000**, 9, 1471-1474	3.5	2
7	Dynamical evolution of the Schottky barrier as a determinant contribution to electron-hole pair stabilization and photocatalysis of plasmon-induced hot carriers.. *Nanoscale*, **2022**,	7.7	2
6	Identification of the Nitrogen Interstitial as Origin of the 3.1 eV Photoluminescence Band in Hexagonal Boron Nitride. *Physica Status Solidi (B): Basic Research*, **2021**, 258, 2100031	1.3	2
5	Density functional tight binding approach utilized to study X-ray-induced transitions in solid materials.. *Scientific Reports*, **2022**, 12, 1551	4.9	1
4	Structural, electronic, and thermodynamic properties of TiO2/organic clusters: performance of DFTB method with different parameter sets. *International Journal of Quantum Chemistry*, **2021**, 121, e26427	2.1	1
3	Using DFTB to Model Photocatalytic Anatase-Rutile TiO Nanocrystalline Interfaces and Their Band Alignment. *Journal of Chemical Theory and Computation*, **2021**, 17, 5239-5247	6.4	0
2	The State of Fortran. *Computing in Science and Engineering*, **2022**, 1-1	1.5	0
1	Accurate Gap Levels and Their Role in the Reliability of Other Calculated Defect Properties **2011**, 139-154		