Eugene Heifets

List of Publications by Year
in descending order

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54 papers	2,794 citations	201385 27 h-index	189595 50 g-index
54 all docs	54 docs citations	54 times ranked	2669 citing authors

#	Article	IF	Citations
1	Bulk properties and electronic structure of SrTiO3, BaTiO3, PbTiO3 perovskites: an ab initio HF/DFT study. Computational Materials Science, 2004, 29, 165-178.	1.4	705
2	Hybrid DFT calculations of the atomic and electronic structure for ABO3 perovskite (001) surfaces. Surface Science, 2005, 575, 75-88.	0.8	177
3	Pathways for Oxygen Incorporation in Mixed Conducting Perovskites: A DFT-Based Mechanistic Analysis for (La, Sr)MnO_{3â^'Î´}. Journal of Physical Chemistry C, 2010, 114, 3017-3027.	1.5	160
4	First-principles calculations for SrTiO3() surface structure. Surface Science, 2002, 513, 211-220.	0.8	120
5	Adsorption of atomic and molecular oxygen on the LaMnO3(001) surface: ab initio supercell calculations and thermodynamics. Physical Chemistry Chemical Physics, 2008, 10, 4644.	1.3	115
6	Semi-empirical simulations of surface relaxation for perovskite titanates. Surface Science, 2000, 462, 19-35.	0.8	113
7	Atomic, electronic and thermodynamic properties of cubic and orthorhombic LaMnO3 surfaces. Surface Science, 2009, 603, 326-335.	0.8	106
8	Electronic structure and thermodynamic stability of double-layeredSrTiO3(001)surfaces:Ab initiosimulations. Physical Review B, 2007, 75, .	1.1	92
9	Electronic structure and thermodynamic stability of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LaMnO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml: <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>La</mml:mtext></mml:mrow><mml:mrow><mml:mn>1</mml:mn> Physical Review B, 2008, 78, .	1.1	85
10	Ab initio DFT+U study of He atom incorporation into UO2 crystals. Physical Chemistry Chemical Physics, 2009, 11, 7241.	1.3	72
11	The first-principles treatment of the electron-correlation and spinâ€“orbital effects in uranium mononitride nuclear fuels. Physical Chemistry Chemical Physics, 2012, 14, 4482.	1.3	70
12	Density functional simulation of theBaZrO3(011) surface structure. Physical Review B, 2007, 75, .	1.1	68
13	Density functional theory calculations on magnetic properties of actinide compounds. Physical Chemistry Chemical Physics, 2010, 12, 12273.	1.3	58
14	Fast oxygen exchange kinetics of pore-free Bi1â^'xSrxFeO3â^'Î´ thin films. Physical Chemistry Chemical Physics, 2011, 13, 16530.	1.3	58
15	Ab initio study of the SrTiO3, BaTiO3 and PbTiO3 (001) surfaces. Ceramics International, 2004, 30, 1989-1992.	2.3	51
16	Calculations for antiferrodistortive phase of SrTiO3perovskite: hybrid density functional study. Journal of Physics Condensed Matter, 2006, 18, 4845-4851.	0.7	51
17	The adhesion nature of the Ag/MgO(100) interface: an ab initio study. Chemical Physics Letters, 1998, 283, 395-401.	1.2	49
18	Ab Initio Study of BiFeO₃: Thermodynamic Stability Conditions. Journal of Physical Chemistry Letters, 2015, 6, 2847-2851.	2.1	48

#	Article	IF	Citations
19	Ab initio calculations of the BaTiO3 (100) and (110) surfaces. Journal of Electroceramics, 2006, 16, 289-292.	0.8	47
20	Ab initio simulation of the BaZrO3 (0 0 1) surface structure. Surface Science, 2007, 601, 490-497.	0.8	43
21	Two types of self-trapped excitons in alkali halide crystals. Physical Review B, 1991, 44, 1499-1508.	1.1	40
22	Calculations of the atomic and electronic structure for SrTiO3 perovskite thin films. Thin Solid Films, 2001, 400, 76-80.	0.8	38
23	Theoretical simulation of localized holes in MgO. Journal of Physics Condensed Matter, 1992, 4, 5711-5722.	0.7	33
24	Modelling of defects and surfaces in perovskite ferroelectrics. Physica Status Solidi (B): Basic Research, 2003, 236, 253-264.	0.7	33
25	Atomistic simulation of the [001]surface structure in BaTiO3. Thin Solid Films, 1997, 296, 76-78.	0.8	30
26	Thermodynamic stability of non-stoichiometric SrFeO_{3â˜Î´}: a hybrid DFT study. Physical Chemistry Chemical Physics, 2019, 21, 3918-3931.	1.3	30
27	Ab initio Hartree-Fock calculations of LaMnO3 (110) surfaces. Solid State Communications, 2003, 127, 367-371.	0.9	29
28	Hartree - Fock simulation of the Ag/MgO interface structure. Journal of Physics Condensed Matter, 1996, 8, 6577-6584.	0.7	27
29	Thermodynamic stability of stoichiometric LaFeO₃ and BiFeO₃: a hybrid DFT study. Physical Chemistry Chemical Physics, 2017, 19, 3738-3755.	1.3	27
30	Atomistic simulation of SrTiO3 and BaTiO3 (110) surface relaxations. Thin Solid Films, 2000, 358, 1-5.	0.8	23
31	Theoretical simulation of VK-centre migration in KCl. I. A quantum-chemical study. Journal of Physics Condensed Matter, 1992, 4, 7417-7428.	0.7	22
32	Atomistic simulation of surface relaxation. Journal of Physics Condensed Matter, 1998, 10, L347-L353.	0.7	22
33	Atomistic simulations of the LaMnO3 (110) polar surface. Physical Chemistry Chemical Physics, 2003, 5, 4180.	1.3	18
34	Theoretical analysis of hole self-trapping in ionic solids: Application to the KCl crystal. Physical Review B, 1993, 47, 14875-14885.	1.1	17
35	The calculation of the self-trapping energy in crystals with mixed valence band. Journal of Physics Condensed Matter, 1992, 4, 8311-8320.	0.7	16
36	The electronic and atomic structure of SrTiO3, BaTiO3, and PbTiO3(001) surfaces: Ab initio DFT/HF hybrid calculations. Microelectronic Engineering, 2005, 81, 472-477.	1.1	16

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37	Electron Tunneling in Quasi-One-Dimensional Resonant Molecular Systems. Ab Initio Study. Journal of Physical Chemistry A, 1998, 102, 2847-2856.	1.1	14
38	Atomistic modeling of polar LaMnO3 surfaces. Sensors and Actuators B: Chemical, 2004, 100, 81-87.	4.0	10
39	Oxygen Incorporation Reaction into Mixed Conducting Perovskites: a Mechanistic Analysis for (La,Sr)MnO₃ Based on DFT Calculations. ECS Transactions, 2009, 25, 2753-2760.	0.3	9
40	Structural Phase Transition and Photo-Charge Carrier Transport in SrTiO3. Ferroelectrics, 2006, 337, 179-188.	0.3	8
41	Calculations of the atomic structure of the KNbO3 (110) surface. Thin Solid Films, 2000, 374, 64-69.	0.8	7
42	Density functional calculations of extended, periodic systems using Coulomb corrected molecular fractionation with conjugated caps method (CC-MFCC). Physical Chemistry Chemical Physics, 2014, 16, 21252-21270.	1.3	7
43	The formulae for calculation of g-tensor shifts in third-order perturbation theory. Chemical Physics, 1992, 160, 363-373.	0.9	5
44	[001] Surface Structure in SrTiO3 â€" Atomistic Study. Surface Review and Letters, 1998, 05, 341-345.	0.5	5
45	First-principles calculations of perovskite thin films. Materials Science in Semiconductor Processing, 2002, 5, 129-134.	1.9	5
46	Adsorption of atomic and molecular oxygen on the SrTiO3(001) surfaces: Computer simulations by means of hybrid density functional calculations and ab initio thermodynamics. Materials Research Society Symposia Proceedings, 2005, 894, 1.	0.1	4
47	First-Principles Modeling of LaMnO3 SOFC Cathode Material. ECS Transactions, 2008, 13, 301-306.	0.3	4
48	Thermodynamics of ABO3-Type Perovskite Surfaces. , 0, , .		4
49	Surface Relaxation in Ferroelectric Perovskites: An Atomistic Study. Materials Research Society Symposia Proceedings, 1996, 459, 219.	0.1	1
50	Computer Modeling of Defects and Surfaces in Advanced Perovskite Ferroelectrics. Japanese Journal of Applied Physics, 2000, 39, 24.	0.8	1
51	Computer Modeling of Point Defects, Impurity Self-Ordering Effects and Surfaces in Advanced Perovskite Ferroelectrics. Acta Physica Polonica A, 2000, 98, 469-481.	0.2	1
52	Program for calculating matrix elements of a semilocal pseudopotential in a Gaussian basis. Journal of Structural Chemistry, 1989, 30, 472-474.	0.3	0
53	Atomistic Study of Surface Polarization in Superconducting Perovskites. Materials Research Society Symposia Proceedings, 1996, 440, 305.	0.1	0
54	Density Functional Theory Calculations On Magnetic Properties Of Actinide Compounds. Materials Research Society Symposia Proceedings, 2011, 1298, 103.	0.1	0