

# Band theory and Mott insulators: HubbardUinstead of S

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Citation Report

#	ARTICLE	IF	CITATIONS
1	Electronic structure of NiO: Correlation and band effects. Physical Review B, 1991, 44, 3604-3626.	1.1	166
2	Many-body electronic structures at transition-metal surfaces: Ni(001). Journal of Physics Condensed Matter, 1992, 4, 9855-9868.	0.7	6
3	Ultraviolet inverse photoemission from iron monoxide and self-interaction-corrected local-spin-density calculations. Physical Review B, 1992, 46, 12165-12174.	1.1	14
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1869	Ab Initio DFT+U Analysis of Oxygen Vacancy Formation and Migration in La <sub>1-x</sub> Sr <sub>x</sub> FeO <sub>3-<math>\delta</math></sub> ( $x=0, 0.25, 0.50$ ). <i>Chemistry of Materials</i> , 2013, 25, 3011-3019.	3.2	153
1871	Incorporation of Nonmetal Impurities at the AnataseTiO <sub>2</sub> (001) $\bar{1}\bar{1}$ (4)Surface. <i>Physical Review Letters</i> , 2013, 110, 016101.	2.9	21
1872	GGA+U studies of the early actinide mononitrides and dinitrides. <i>Journal of Nuclear Materials</i> , 2013, 442, 235-244.	1.3	33
1873	Massive Symmetry Breaking in LaAlO <sub>3</sub> stretched on Si(111). <i>Physical Review Letters</i> , 2013, 111, 126804.		
1874	Implementation of the modified Becke-Johnson meta-GGA functional in Quantum Espresso. <i>Computer Physics Communications</i> , 2013, 184, 1697-1700.	3.0	19
1875	Simultaneous Etching and Doping of TiO <sub>2</sub> Nanowire Arrays for Enhanced Photoelectrochemical Performance. <i>ACS Nano</i> , 2013, 7, 9375-9383.	7.3	152
1876	Vacancy and doping driven ferromagnetism in BaTiO <sub>3</sub> perovskite. <i>Physica B: Condensed Matter</i> , 2013, 424, 79-83.	1.3	26



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1877	Stable platinum nanoparticles on specific MgAl <sub>2</sub> O <sub>4</sub> spinel facets at high temperatures in oxidizing atmospheres. Nature Communications, 2013, 4, 2481.	5.8	166
1878	Application to paramagnetic phases of UO <sub>2</sub> modeling of actinide-based alloys: Origin of giant spin-lattice coupling and the suppression of ferroelectricity in EuTiO <sub>3</sub> from first principles. Physical Review B, 2013, 87, .	1.1	57
1879	Origin of giant spin-lattice coupling and the suppression of ferroelectricity in EuTiO <sub>3</sub> from first principles. Physical Review B, 2013, 88, .	1.1	45
1880	Infrared spectroscopy and the ferromagnetic transition in Gd. Journal of Physics Condensed Matter, 2013, 25, 036002.	0.7	0
1881	Enhance ferromagnetism by stabilizing the cation vacancies in GaN. European Physical Journal B, 2013, 86, 1.	0.6	7
1882	Symmetry-induced quantum interference effects in metalloporphyrin wires. Journal of Physics Condensed Matter, 2013, 25, 325501.	0.7	7
1883	Correlated Electron Materials and Field Effect Transistors for Logic: A Review. Critical Reviews in Solid State and Materials Sciences, 2013, 38, 286-317.	6.8	100
1884	High-efficiently visible light-responsive photocatalysts: Ag <sub>3</sub> PO <sub>4</sub> tetrahedral microcrystals with exposed {111} facets of high surface energy. Journal of Materials Chemistry A, 2013, 1, 12635.	5.2	100
1885	Oxide ion transport in Sr <sub>2</sub> Fe <sub>1.5</sub> Mo <sub>0.5</sub> O <sub>6-<math>\delta</math></sub> , a mixed ion-electron conductor: new insights from first principles modeling. Physical Chemistry Chemical Physics, 2013, 15, 6250.	1.3	59
1886	Topological insulators from the perspective of first-principles calculations. Physica Status Solidi - Rapid Research Letters, 2013, 7, 72-81.	1.2	70
1887	Defect states and excitations in a Mott insulator with orbital degrees of freedom: Mott-Hubbard gap versus optical and transport gaps in doped systems. Physical Review B, 2013, 87, .	1.1	23
1888	Electronic structures of compensated magnetism in double perovskites A <sub>2</sub> CrRu(Os)O <sub>6</sub> (A=Si, Ge, Sn,) Tj ETQq1 1 0,784314 rgBT /Over	2.8	13
1889	Structural stability, band structure and magnetic properties of ZnS and Zn <sub>0.75</sub> Cr <sub>0.25</sub> S under pressure. Journal of Alloys and Compounds, 2013, 549, 184-189.	2.8	13
1890	Validation of binuclear descriptor for mixed transition metal oxide supported electrocatalytic water oxidation. Catalysis Today, 2013, 202, 114-119.	2.2	32
1891	Thermoelectric properties of Tl <sub>1-x</sub> Ln <sub>x</sub> Te <sub>6</sub> , with Ln=Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho and Er, and 0.25x <sup>1/2</sup> 1.32. Journal of Alloys and Compounds, 2013, 549, 126-134.	2.8	26
1892	Electronic Origin of the Surface Reactivity of Transition-Metal-Doped TiO <sub>2</sub> (110). Journal of Physical Chemistry C, 2013, 117, 460-465.	1.5	87
1893	Density Functional Theory Studies of the Electronic Structure of Solid State Actinide Oxides. Chemical Reviews, 2013, 113, 1063-1096.	23.0	191
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1897	Undoped visible-light-sensitive titania photocatalyst. <i>Journal of Materials Science</i> , 2013, 48, 108-114.	1.7	30
1898	Transition metal oxide alloys as potential solar energy conversion materials. <i>Journal of Materials Chemistry A</i> , 2013, 1, 2474.	5.2	63
1899	Ab initio study of ZnCoO diluted magnetic semiconductor and its magnetic properties. <i>Journal of Alloys and Compounds</i> , 2013, 551, 306-311.	2.8	19
1900	New concepts and modeling strategies to design and evaluate photo-electro-catalysts based on transition metal oxides. <i>Chemical Society Reviews</i> , 2013, 42, 2401-2422.	18.7	225
1901	Ti <sub>0.89</sub> Si <sub>0.11</sub> O <sub>2</sub> single crystals bound by high-index {201} facets showing enhanced visible-light photocatalytic hydrogen evolution. <i>Chemical Communications</i> , 2013, 49, 2016.	2.2	25
1902	Structure Sensitivity of CO Oxidation on Co <sub>3</sub> O <sub>4</sub> : A DFT Study. <i>ChemPhysChem</i> , 2013, 14, 204-212.	1.0	64
1903	Interstitial hydrogen in ZnO and BeZnO. <i>International Journal of Hydrogen Energy</i> , 2013, 38, 5974-5982.	3.8	9
1904	On the delithiation mechanism of Li <sub>2</sub> FeSiO <sub>4</sub> -y <sub>2</sub> Sy compounds: A first-principles investigation. <i>Electrochimica Acta</i> , 2013, 112, 670-677.	2.6	14
1905	Density functional studies of selected metal dioxides. <i>Journal of Physics and Chemistry of Solids</i> , 2013, 74, 1632-1639.	1.9	15
1906	First principle research of possible HM-AFM in double perovskites A <sub>2</sub> MoOsO <sub>6</sub> and A <sub>2</sub> TcReO <sub>6</sub> (A=Si, Ge). <i>TJ ETQq</i> 1.1 0.784314 rgBT (C)	1.5	2
1907	Study of the half-metallic materials double perovskites Sr <sub>2</sub> ZnBO <sub>6</sub> (B=Tc, Re, Ru, Os, Co, Pd, and Au) via first-principle calculations. <i>Journal of Magnetism and Magnetic Materials</i> , 2013, 341, 25-29.	1.0	25
1908	Role of Oxygen Vacancies in Catalytic SO <sub>3</sub> Decomposition over Cu <sub>2</sub> V <sub>2</sub> O <sub>7</sub> in Solar Thermochemical Water Splitting Cycles. <i>Journal of Physical Chemistry C</i> , 2013, 117, 26710-26715.	1.5	33
1909	Atomic-Scale Engineering of the Electrostatic Landscape of Semiconductor Surfaces. <i>Nano Letters</i> , 2013, 13, 2418-2422.	4.5	15
1910	Ab Initio Prediction of Surface Stability of Fluorite Materials and Experimental Verification. <i>Journal of Physical Chemistry C</i> , 2013, 117, 6639-6650.	1.5	24
1911	Implication of volume changes in uranium oxides: A density functional study. <i>Solid State Sciences</i> , 2013, 24, 44-53.	1.5	13
1912	First-principles calculations of structural, magnetic phase stability and electronic properties of RVO <sub>4</sub> compounds. <i>Computational Materials Science</i> , 2013, 68, 361-366.	1.4	13

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1916	First-principle study of amorphous SiZnSnO thin-film transistor with excellent stability. Thin Solid Films, 2013, 534, 609-613.	0.8	29
1917	Magnetic ordering and electron correlation of iron-based superconductor (Ca <sub>3</sub> Al <sub>2</sub> O <sub>5</sub> ~x)(Fe <sub>2</sub> As <sub>2</sub> ) from first-principles study. Solid State Communications, 2013, 172, 41-48.	0.9	0
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1920	Density functionals and model Hamiltonians: Pillars of many-particle physics. Physics Reports, 2013, 528, 91-159.	10.3	77
1921	Band structure and phase stability of the copper oxides Cu <sub>2</sub> O, CuO, and Cu <sub>4</sub> O. Physical Review B, 2013, 87, .	1.1	309
1922	A combination of multiple chromophores enhances second-harmonic generation in a nonpolar noncentrosymmetric oxide: CdTeMoO <sub>6</sub> . Journal of Materials Chemistry C, 2013, 1, 2906.	2.7	67
1923	DFT+U Investigation of Propene Oxidation over Bismuth Molybdate: Active Sites, Reaction Intermediates, and the Role of Bismuth. Journal of Physical Chemistry C, 2013, 117, 7123-7137.	1.5	70
1924	Catalysis by Doped Oxides. Chemical Reviews, 2013, 113, 4391-4427.	23.0	687
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1927	Massive Dirac surface states in topological insulator/magnetic insulator heterostructures. Physical Review B, 2013, 87, .	1.1	132
1928	Electronic structure and magnetic properties of CrSb <sub>2</sub> and FeSb <sub>2</sub> investigated via ab initio calculations. Physical Review B, 2013, 87, .	1.1	14
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1932	Charging of Gold Atoms on Doped MgO and CaO: Identifying the Key Parameters by DFT Calculations. Journal of Physical Chemistry C, 2013, 117, 9943-9951.	1.5	45
1933	Electronic interactions and charge transfers of metal atoms and clusters on oxide surfaces. Physical Chemistry Chemical Physics, 2013, 15, 1737.	1.3	203
1934	Surface structure and equilibrium particle shape of the LiMn <sub>2</sub> O <sub>4</sub> spinel from first-principles calculations. Physical Review B, 2013, 87, .	1.1	116
1935	Visible-light-responsive copper(II) borate photocatalysts with intrinsic midgap states for water splitting. Journal of Materials Chemistry A, 2013, 1, 1553-1556.	5.2	38
1936	Phase equilibria of (Mg,Fe)2SiO4 at the Earth's upper mantle conditions from first-principles studies. Physics of the Earth and Planetary Interiors, 2013, 217, 36-47.	0.7	8
1937	Density-Functional Theory of Free and Supported Metal Nanoclusters and Nanoalloys. Nanostructure Science and Technology, 2013, , 29-79.	0.1	7
1938	DFT+U Study of Molecular and Dissociative Water Adsorptions on the Fe <sub>3</sub> O <sub>4</sub> (110) Surface. Journal of Physical Chemistry C, 2013, 117, 7648-7655.	1.5	46
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1941	Role of screening in the density functional applied to transition-metal defects in semiconductors. Physical Review B, 2013, 87, .	1.1	35
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1945	Crystal structure analysis and first principle investigation of F doping in LiFePO4. Journal of Power Sources, 2013, 241, 70-79.	4.0	42
1946	Electronic structure of substitutional group-1B impurities in $\beta$ -Silicon carbide. Chemical Physics Letters, 2013, 578, 59-65.	1.2	1
1947	Sum rule violation in self-consistent hybridization expansions. Physical Review B, 2013, 87, .	1.1	15
1948	Correlation effects on the electronic structure of Co2Mn0.5Fe0.5Si and Co2Mn0.5Gd0.5Si quaternary alloys. Intermetallics, 2013, 37, 27-31.	1.8	6
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1952	Cation and magnetic orders in MnFe <sub>2</sub> O <sub>4</sub> from density functional calculations. Journal of Applied Physics, 2013, 113, .	1.1	46
1953	Ruthenia-Based Electrochemical Supercapacitors: Insights from First-Principles Calculations. Accounts of Chemical Research, 2013, 46, 1084-1093.	7.6	67
1954	Water adsorption and dissociation on $\hat{\pm}$ -Fe <sub>2</sub> O <sub>3</sub> (0001): PBE+U calculations. Journal of Chemical Physics, 2013, 138, 194709.	1.2	105
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1962	Relative stability of normal vs. inverse spinel for 3d transition metal oxides as lithium intercalation cathodes. Physical Chemistry Chemical Physics, 2013, 15, 6486.	1.3	42
1963	Ab initio study of the fracture energy of LiFePO <sub>4</sub> /FePO <sub>4</sub> interfaces. Journal of Power Sources, 2013, 243, 706-714.	4.0	21
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1971	Correlation effects in the electronic structure of the Ni-based superconducting $KNi_2S$ . Physical Review B, 2013, 87, .	1.1	6
1972	Plasmon Absorption of Au-in-CoAl <sub>2</sub> O <sub>4</sub> Linear Nanopeapod Chains. Journal of Physical Chemistry C, 2013, 117, 14142-14148.	1.5	20
1973	Oxygen Defects and Surface Chemistry of Ceria: Quantum Chemical Studies Compared to Experiment. Chemical Reviews, 2013, 113, 3949-3985.	23.0	849
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1977	A first-principles comparative study of exchange and correlation potentials for ZnO. Materials Science in Semiconductor Processing, 2013, 16, 1162-1169.	1.9	39
1978	Structure-Property Relationship and Chemical Aspects of Oxide-Metal Hybrid Nanostructures. Chemical Reviews, 2013, 113, 4314-4372.	23.0	160
1979	Electronic Band Gap Reduction in Manganese Carbodiimide: MnNCN. Journal of Physical Chemistry C, 2013, 117, 12754-12761.	1.5	36
1980	Theoretical assessment on the possibility of constraining point-defect energetics by pseudo phase transition pressures. Physical Review B, 2013, 87, .	1.1	1
1981	AgBr Nanocrystals from Plates to Cubes and Their Photocatalytic Properties. ChemCatChem, 2013, 5, 1426-1430.	1.8	13
1982	On Pair Functions for Strong Correlations. Journal of Chemical Theory and Computation, 2013, 9, 2857-2869.	2.3	24
1983	Enhanced magnetization and conductive phase in NiFe <sub>2</sub> O <sub>4</sub> . Journal of Magnetism and Magnetic Materials, 2013, 325, 144-146.	1.0	18
1984	Quantum mechanical method for estimating ionicity of spinel ferrites. Journal of Magnetism and Magnetic Materials, 2013, 326, 197-200.	1.0	41
1985	Hydroxylation-induced surface stability of AnO <sub>2</sub> (An=U, Np, Pu) from first-principles. Surface Science, 2013, 608, 180-187.	0.8	59

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1987	First Principles Study of Cobalt (Hydr)oxides under Electrochemical Conditions. Journal of Physical Chemistry C, 2013, 117, 20002-20006.	1.5	89
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1993	Water Adsorption at the Tetrahedral Titania Surface Layer of SrTiO <sub>3</sub> (110)-(4 Å <sup>-1</sup> ). Journal of Physical Chemistry C, 2013, 117, 26060-26069.	1.5	32
1994	Microscopic theory of the insulating electronic ground states of the actinide dioxides AnO <sub>2</sub> ( $(An^{\%}U, Np, Tj) ETQq 0 0 rgBT$ )	1.1	58
1995	Electronic structures and thermoelectric properties of layered BiCuOCh oxychalcogenides (Ch = S, Tj ETQq 1 1 0.784314 rgBT /Overlo	5.2	128
1996	Origin of the Visible Light Absorption of Boron/Nitrogen Co-doped Anatase TiO <sub>2</sub> . Journal of Physical Chemistry C, 2013, 117, 26454-26459.	1.5	25
1997	Dielectric constant of NiO and LDA $U$ Physical Review B, 2013, 87, .		
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2002	Exploring highly correlated materials via electron pair emission: the case of NiO/Ag(100). Journal of Physics Condensed Matter, 2013, 25, 094002.	0.7	8
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2005	STRUCTURAL AND MAGNETIC PHASE TRANSITIONS OF $\text{BiFeO}_3$ INDUCED BY PRESSURE. Functional Materials Letters, 2013, 06, 1350026.	0.7	1
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2021	Orbital Localization, Charge Transfer, and Band Gaps in Semilocal Density-Functional Theory. Physical Review Letters, 2013, 111, 036402.	2.9	78
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