Yoyo Hinuma

List of Publications by Citations

23 papers	755 citations	11 h-index	25 g-index
25 ext. papers	992 ext. citations	4.6 avg, IF	4.41 L-index

#	Paper	IF	Citations
23	Band structure diagram paths based on crystallography. *Computational Materials Science*, **2017**, 128, 140-184	3.2	247
22	Band alignment of semiconductors from density-functional theory and many-body perturbation theory. *Physical Review B*, **2014**, 90,	3.3	203
21	Comparison of approximations in density functional theory calculations: Energetics and structure of binary oxides. *Physical Review B*, **2017**, 96,	3.3	58
20	Density Functional Theory Calculations of Oxygen Vacancy Formation and Subsequent Molecular Adsorption on Oxide Surfaces. *Journal of Physical Chemistry C*, **2018**, 122, 29435-29444	3.8	51
19	Band offsets of CuInSe2/CdS and CuInSe2/ZnS (110) interfaces: A hybrid density functional theory study. *Physical Review B*, **2013**, 88,	3.3	38
18	Categorization of surface polarity from a crystallographic approach. *Computational Materials Science*, **2016**, 113, 221-230	3.2	31
17	Band alignment at surfaces and heterointerfaces of Al2O3, Ga2O3, In2O3, and related group-III oxide polymorphs: A first-principles study. *Physical Review Materials*, **2019**, 3,	3.2	18
16	Effects of composition, crystal structure, and surface orientation on band alignment of divalent metal oxides: A first-principles study. *Physical Review Materials*, **2018**, 2,	3.2	16
15	Finding a junction partner for candidate solar cell absorbers enargite and bournonite from electronic band and lattice matching. *Journal of Applied Physics*, **2019**, 125, 055703	2.5	13
14	Linear Correlations between Adsorption Energies and HOMO Levels for the Adsorption of Small Molecules on TiO2 Surfaces. *Journal of Physical Chemistry C*, **2019**, 123, 20988-20997	3.8	13
13	Frontier Molecular Orbital Based Analysis of Solid□Adsorbate Interactions over Group 13 Metal Oxide Surfaces. *Journal of Physical Chemistry C*, **2020**, 124, 15355-15365	3.8	12
12	Surface Oxygen Vacancy Formation Energy Calculations in 34 Orientations of □Ga2O3 and □Al2O3. *Journal of Physical Chemistry C*, **2020**, 124, 10509-10522	3.8	11
11	Valence band offsets at zinc-blende heterointerfaces with misfit dislocations: A first-principles study. *Physical Review B*, **2013**, 88,	3.3	10
10	Changes in Surface Oxygen Vacancy Formation Energy at Metal/Oxide Perimeter Sites: A Systematic Study on Metal Nanoparticles Deposited on an In2O3(111) Support. *Journal of Physical Chemistry C*, **2020**, 124, 27621-27630	3.8	10
9	The effect of cation size on hydride-ion conduction in LnSrLiH2O2 (Ln = La, Pr, Nd, Sm, Gd) oxyhydrides. *Journal of Materials Chemistry A*, **2020**, 8, 24685-24694	13	5
8	Surface activation by electron scavenger metal nanorod adsorption on TiH, TiC, TiN, and TiO. *Physical Chemistry Chemical Physics*, **2021**, 23, 16577-16593	3.6	5
7	Factors determining surface oxygen vacancy formation energy in ternary spinel structure oxides with zinc. *Physical Chemistry Chemical Physics*, **2021**, 23, 23768-23777	3.6	5

List of Publications

6	Effect of Oxygen Vacancies on Adsorption of Small Molecules on Anatase and Rutile TiO2 Surfaces: A Frontier Orbital Approach. *Journal of Physical Chemistry C*, **2021**, 125, 3827-3844	3.8	3
5	A simplified methodology for the modeling of interfaces of elementary metals. *AIP Advances*, **2021**, 11, 115020	1.5	2
4	Reactions of the LiMnO Cathode in an All-Solid-State Thin-Film Battery during Cycling. *ACS Applied Materials & Interfaces*, **2021**, 13, 7650-7663	9.5	1
3	Understanding and controlling the formation of surface anion vacancies for catalytic applications. *Catalysis Science and Technology*, **2022**, 12, 2398-2410	5.5	0
2	Experimental and Theoretical Investigation of Metal–Support Interactions in Metal-Oxide-Supported Rhenium Materials. *Journal of Physical Chemistry C*, **2022**, 126, 4472-4482	3.8	0
1	Categorization of inorganic crystal structures by Delaunay tetrahedralization. *Science and Technology of Advanced Materials Methods*, **2022**, 2, 75-83		