Eunja Kim

List of Publications by Citations

56 papers	864 citations	19 h-index	27 g-index
56 ext. papers	970 ext. citations	3.7 avg, IF	4.31 L-index

#	Paper	IF	Citations
56	Structural, electronic, and vibrational properties of liquid and amorphous silicon: Tight-binding molecular-dynamics approach. *Physical Review B*, **1994**, 49, 1743-1749	3.3	61
55	Structures of uranyl peroxide hydrates: a first-principles study of studtite and metastudtite. *Dalton Transactions*, **2012**, 41, 9748-52	4.3	50
54	On the mechanical stability of uranyl peroxide hydrates: implications for nuclear fuel degradation. *RSC Advances*, **2015**, 5, 79090-79097	3.7	41
53	Cubic phases of BC2N: A first-principles study. *Physical Review B*, **2007**, 75,	3.3	40
52	Solar Energy Storage in Phase Change Materials: First-Principles Thermodynamic Modeling of Magnesium Chloride Hydrates. *Journal of Physical Chemistry C*, **2014**, 118, 4618-4625	3.8	38
51	Mechanical properties of zirconium alloys and zirconium hydrides predicted from density functional perturbation theory. *Dalton Transactions*, **2015**, 44, 18769-79	4.3	37
50	First-principles study of phase stability of BN under pressure. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2003**, 319, 384-389	2.3	34
49	Layered uranium(VI) hydroxides: structural and thermodynamic properties of dehydrated schoepite □UO□(OH)□ *Dalton Transactions*, **2014**, 43, 17191-9	4.3	33
48	Nanoscale building blocks for the development of novel proton exchange membrane fuel cells. *Journal of Physical Chemistry B*, **2008**, 112, 3283-6	3.4	33
47	Pressure-driven phase transitions in NaBH4: theory and experiments. *Journal of Physical Chemistry B*, **2007**, 111, 13873-6	3.4	32
46	On the role of strong electron correlations in the surface properties and chemistry of uranium dioxide. *Dalton Transactions*, **2013**, 42, 4570-8	4.3	31
45	Mechanism of fullerene hydrogenation by polyamines: Ab initio density functional calculations. *Physical Review B*, **2008**, 78,	3.3	28
44	Martensitic fcc-to-hcp transformations in solid xenon under pressure: a first-principles study. *Physical Review Letters*, **2006**, 96, 035504	7.4	28
43	Uncloaking the Thermodynamics of the Studtite to Metastudtite Shear-Induced Transformation. *Journal of Physical Chemistry C*, **2016**, 120, 16553-16560	3.8	28
42	Relationship between crystal structure and thermo-mechanical properties of kaolinite clay: beyond standard density functional theory. *Dalton Transactions*, **2015**, 44, 12550-60	4.3	26
41	Tetragonal crystalline carbon nitrides: theoretical predictions. *Physical Review Letters*, **2001**, 86, 652-5	7.4	26
40	Magic numbers in small iron clusters: A first-principles study. *Chemical Physics Letters*, **2014**, 613, 59-63	2.5	23

39	Calculation of bulk modulus for highly anisotropic materials. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2004**, 326, 442-448	2.3	23
38	Electronic structure of vacancies in amorphous silicon. *Physical Review B*, **1995**, 51, 5429-5432	3.3	21
37	Assessing Hubbard-corrected AM05+U and PBEsol+U density functionals for strongly correlated oxides CeO and CeO. *Physical Chemistry Chemical Physics*, **2016**, 18, 26816-26826	3.6	19
36	Structural and magnetic properties of Tcn@C60 endohedral metalofullerenes: First-principles predictions. *Physical Review B*, **2010**, 81,	3.3	18
35	Interplay between structure, stoichiometry and properties of technetium nitrides. *Dalton Transactions*, **2011**, 40, 6738-44	4.3	18
34	Pressure-Tuneable Visible-Range Band Gap in the Ionic Spinel Tin Nitride. *Angewandte Chemie - International Edition*, **2018**, 57, 11623-11628	16.4	16
33	Density functional analysis of the trigonal uranyl equatorial coordination in hexahomotrioxacalix[3]arene-based macrocyclic complexes. *Inorganic Chemistry*, **2010**, 49, 1465-70	5.1	14
32	Model representations of kerogen structures: An insight from density functional theory calculations and spectroscopic measurements. *Scientific Reports*, **2017**, 7, 7068	4.9	13
31	Thermodynamics of technetium: reconciling theory and experiment using density functional perturbation analysis. *Dalton Transactions*, **2015**, 44, 12735-42	4.3	11
30	High-pressure studies of 1,3,5,7-cyclooctatetraene: experiment and theory. *Journal of Physical Chemistry A*, **2008**, 112, 11501-7	2.8	11
29	Infrared and Raman spectroscopy of □ZrW2O8: A comprehensive density functional perturbation theory and experimental study. *Journal of Raman Spectroscopy*, **2018**, 49, 1373-1384	2.3	8
28	Phosphorus Dimerization in Gallium Phosphide at High Pressure. *Inorganic Chemistry*, **2018**, 57, 2432-2437	4.7	7
27	Technetium incorporation in scheelite: insights from first-principles. *Dalton Transactions*, **2016**, 45, 18171-18176	4.3	7
26	Density Functional Analysis of Fluorite-Structured (Ce, Zr)O2/CeO2 Interfaces. *Journal of Physical Chemistry C*, **2017**, 121, 14678-14687	3.8	7
25	Nuclear forward scattering and first-principles studies of the iron oxide phase Fe4O5. *Physical Review B*, **2014**, 90,	3.3	7
24	Characterization of pentavalent and hexavalent americium complexes in nitric acid using X-ray absorption fine structure spectroscopy and first-principles modeling. *Journal of Radioanalytical and Nuclear Chemistry*, **2016**, 309, 1087-1095	1.5	7
23	Synthesis of a novel strontium-based wide-bandgap semiconductor via X-ray photochemistry under extreme conditions. *Journal of Materials Chemistry C*, **2018**, 6, 12473-12478	7.1	7
22	First-Principles Structural, Mechanical, and Thermodynamic Calculations of the Negative Thermal Expansion Compound Zr(WO)(PO). *ACS Omega*, **2018**, 3, 15780-15788	3.9	7

21	Assessing exchange-correlation functionals for elasticity and thermodynamics of ZrW2O8: A density functional perturbation theory study. *Chemical Physics Letters*, **2018**, 698, 195-199	2.5	6
20	Organic cyclic difluoramino-nitramines: infrared and Raman spectroscopy of 3,3,7,7-tetrakis(difluoramino)octahydro 1,5-dinitro-1,5-diazocine (HNFX). *Journal of Raman Spectroscopy*, **2009**, 40, 964-971	2.3	6
19	Reverse-martensitic hcp-to-fcc transformation in technetium under shock compression. *Journal of Applied Physics*, **2018**, 124, 035903	2.5	5
18	Lattice dynamics and thermomechanical properties of zirconium(IV) chloride: Evidence for low-temperature negative thermal expansion. *Chemical Physics Letters*, **2018**, 691, 98-102	2.5	5
17	Diperoxo Pertechnetic Acid Characterized by Spectroscopic and Quantum Chemical Studies. *European Journal of Inorganic Chemistry*, **2013**, 2013, 4595-4600	2.3	4
16	Equation of state for technetium from X-ray diffraction and first-principle calculations. *Journal of Physics and Chemistry of Solids*, **2016**, 95, 6-11	3.9	4
15	Dimer-Exchange Mechanism in Surfactant-Mediated Si/Ge Epitaxial Growth. *Journal of Physical Chemistry B*, **2002**, 106, 891-894	3.4	3
14	Crystal and Electronic Structures of ANaIO Periodate Double Perovskites (A = Sr, Ca, Ba): Candidate Wasteforms for I-129 Immobilization. *Inorganic Chemistry*, **2020**, 59, 18407-18419	5.1	3
13	Structure-thermodynamics relationship of schoepite from first-principles. *Physical Chemistry Chemical Physics*, **2019**, 21, 25569-25576	3.6	3
12	Pressure-Tuneable Visible-Range Band Gap in the Ionic Spinel Tin Nitride. *Angewandte Chemie*, **2018**, 130, 11797-11802	3.6	3
11	Interaction of cesium adatoms with free-standing graphene and graphene-veiled SiO2 surfaces. *RSC Advances*, **2015**, 5, 38623-38629	3.7	2
10	Speciation of technetium peroxo complexes in sulfuric acid revisited. *Journal of Radioanalytical and Nuclear Chemistry*, **2015**, 303, 1163-1167	1.5	2
9	Structural Relaxation of Vacancies in Amorphous Silicon. *Materials Research Society Symposia Proceedings*, **1997**, 467, 555		2
8	Zirconium tetrachloride revisited. *Acta Crystallographica Section C, Structural Chemistry*, **2018**, 74, 307-311	0.8	2
7	Zirconium chloride molecular species: combining electron impact mass spectrometry and first principles calculations. *SN Applied Sciences*, **2019**, 1, 1	1.8	1
6	A comprehensive assessment of the low-temperature thermal properties and thermodynamic functions of CeO. *Journal of Chemical Physics*, **2019**, 151, 044202	3.9	1
5	X-ray Crystallographic and First-Principles Theoretical Studies of K2[TcOCl5] and UV/Vis Investigation of the [TcOCl5]2− and [TcOCl4]− Ions. *European Journal of Inorganic Chemistry*, **2013**, 2013, 1097-1104	2.3	1
4	Radionuclide incorporation in negative thermal expansion Zr(WO4)2: A density functional theory study. *Chemical Physics Letters*, **2020**, 744, 137172	2.5	1

List of Publications

3	Thermodynamic properties of metaschoepite predicted from density functional perturbation theory. *Chemical Physics Letters*, **2020**, 757, 137878	2.5	0
2	Energetics of Sn2+ isomorphic substitution into hydroxylapatite: first-principles predictions. *RSC Advances*, **2016**, 6, 107286-107292	3.7	0
1	Transferable Tight-Binding Approach Of Si-H Interactions. *Materials Research Society Symposia Proceedings*, **1997**, 491, 347		