## Hasan HÃ<sup>1</sup>/<sub>4</sub>seyin Kart

List of Publications by Year in descending order

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567144 610775 26 577 15 24 g-index citations h-index papers 26 26 26 543 docs citations times ranked citing authors all docs

#	Article	IF	Citations
1	Elastic properties and pressure induced transitions of ZnO polymorphs from first-principle calculations. Journal of Alloys and Compounds, 2009, 484, 431-438.	2.8	85
2	Physical properties of Cu nanoparticles: A molecular dynamics study. Materials Chemistry and Physics, 2014, 147, 204-212.	2.0	72
3	Thermodynamical and mechanical properties of Pd–Ag alloys. Computational Materials Science, 2005, 32, 107-117.	1.4	50
4	Thermal and mechanical properties of Cu–Au intermetallic alloys. Modelling and Simulation in Materials Science and Engineering, 2005, 13, 657-669.	0.8	36
5	DFT studies of sulfur induced stress corrosion cracking in nickel. Computational Materials Science, 2009, 44, 1236-1242.	1.4	35
6	A combined experimental and DFT investigation of disazo dye having pyrazole skeleton. Journal of Molecular Structure, 2017, 1129, 222-230.	1.8	32
7	B3–B1 phase transition and pressure dependence of elastic properties of ZnS. Materials Chemistry and Physics, 2008, 111, 559-564.	2.0	30
8	High pressure phase transitions in SnO2 polymorphs by first-principles calculations. Journal of Alloys and Compounds, 2014, 587, 638-645.	2.8	29
9	Synthesis, crystal structure and ab initio/DFT calculations of a derivative of dithiophosphonates. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 122, 582-590.	2.0	21
10	New coumarin-based disperse disazo dyes: Synthesis, spectroscopic properties and theoretical calculations. Journal of Molecular Liquids, 2016, 223, 557-565.	2.3	21
11	MOLECULAR DYNAMICS STUDY OF THE COALESCENCE OF EQUAL AND UNEQUAL SIZED <font>Cu</font> NANOPARTICLES. International Journal of Modern Physics C, 2009, 20, 179-196.	0.8	20
12	Theoretical study of the structure–properties relationship in new class of 2,5-di(2-thienyl)pyrrole compounds. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 137, 1174-1183.	2.0	18
13	Synthesis and DFT calculation of a novel 5,17-di(2-antracenylazo)-25,27-di(ethoxycarbonylmethoxy)-26,28-dihydroxycalix[4]arene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 607-617.	2.0	18
14	Ab initio studies of NMR chemical shifts for calix[4] arene and its derivatives. Structural Chemistry, 2009, 20, 113-119.	1.0	17
15	Simulation of crystallization and glass formation of binary Pd–Ag metal alloys. Journal of Non-Crystalline Solids, 2004, 342, 6-11.	1.5	16
16	Ab initio/DFT calculations of butyl ammonium salt of O,O′-dibornyl dithiophosphate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 129, 421-428.	2.0	13
17	Quantum mechanical calculations of different monomeric structures with the same electroactive group to clarify the relationship between structure and ultimate optical and electrochemical properties of their conjugated polymers. Journal of Physics and Chemistry of Solids, 2021, 149, 109720.	1.9	10
18	STRUCTURAL AND DYNAMICAL PROPERTIES OF LIQUID PD–AG ALLOYS. International Journal of Modern Physics B, 2004, 18, 2257-2269.	1.0	9

#	Article	IF	CITATIONS
19	Atomic-scale insights into structural and thermodynamic stability of spherical Al@Ni and Ni@Al core–shell nanoparticles. Journal of Nanoparticle Research, 2020, 22, 1.	0.8	9
20	Synthesis and structural study on (1E,2E,1′E,2′E)-3,3′-bis[(4-bromophenyl)-3,3′-(4-methy-1,2-phenyle Spectroscopy (English Translation of Optika I Spektroskopiya), 2015, 118, 865-881.	ne) Tj ETQ 0.2	q0 0 0 rgBT / 8
21	Synthesis and characterization of three novel Schiff base compounds: Experimental and theoretical study. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2015, 119, 467-484.	0.2	8
22	First principles lattice dynamics study of SnO2 polymorphs. Journal of Alloys and Compounds, 2015, 633, 272-279.	2.8	7
23	Synthesis and investigation of the properties of novel azocalix[4]arenes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 146, 151-162.	2.0	6
24	Density functional theory study of tin and titanium dioxides: Structural and mechanical properties in the tetragonal rutile phase. Materials Science in Semiconductor Processing, 2014, 28, 59-65.	1.9	4
25	Theoretical investigations on HgTe chalcogenide materials under high pressure. Physica Scripta, 2021, 96, 045703.	1.2	3
26	The analysis of the stress corrosion effects for H atom in the symmetrical tilt Ni $\hat{l}$ £ 5 (012) grain boundary structure. Materials Today: Proceedings, 2017, 4, 7011-7017.	0.9	0