Alexis Markovits

List of Publications by Year
in descending order

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26	543	687363 13	642732 23
papers	citations	h-index	g-index

27	27	27	811
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Peculiar adsorption induced by strong hydrogen bonds on perfect anatase (0 0 1) surface. Applied Surface Science, 2022, 594, 153397.	6.1	2
2	Reactivity of transition metal atoms supported or not on TiO2(110) toward CO and H adsorption. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	4
3	Metal atom adsorption on a defective TiO2â€“x support. Chemical Physics Letters, 2014, 594, 23-29.	2.6	5
4	Exploring CO dissociation on Fe nanoparticles by density functional theory-based methods: Fe13 as a case study. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	7
5	CO dissociation on magnetic Fe_n clusters. Physical Chemistry Chemical Physics, 2014, 16, 20703-20713.	2.8	16
6	Support effect on H adsorption on a metal atom. Chemical Physics Letters, 2013, 565, 45-51.	2.6	6
7	Core restructuring for magnetic Fe55 icosahedral nanoparticles. Chemical Physics Letters, 2012, 541, 101-104.	2.6	10
8	First-row transition metal atoms adsorption on rutile TiO2(110) surface. Structural Chemistry, 2012, 23, 1309-1321.	2.0	17
9	Triethylamine on Si(001)-(2 Ã— 1) at 300 K: Molecular Adsorption and Site Configurations Leading to Dissociation. Journal of Physical Chemistry C, 2012, 116, 16473-16486.	3.1	26
10	Improved convergence of rutile-TiO2(110) slab properties with thickness by one-side saturation. Chemical Physics Letters, 2012, 531, 90-93.	2.6	5
11	Modeling Localized Photoinduced Electrons in Rutile-TiO₂ Using Periodic DFT+U Methodology. Langmuir, 2010, 26, 16232-16238.	3.5	36
12	Increased CO adsorption on supported VIB and IB metals. Chemical Physics Letters, 2009, 475, 215-219.	2.6	2
13	Adsorption of the first row of transition metals on the perfect and defective MgO(100) surface. Chemical Physics Letters, 2008, 463, 106-111.	2.6	17
14	Coadsorption of Gold with Hydrogen or Potassium on TiO2(110) Surface. Journal of Physical Chemistry C, 2008, 112, 14010-14014.	3.1	13
15	First Row Transition Metal Atom Adsorption On-Top of FÂ°_s Defects of a MgO(100) Surface. Journal of Physical Chemistry C, 2008, 112, 16491-16496.	3.1	13
16	First Row Transition Metal Atom Adsorption on Defect-Free MgO(100) Surface. Journal of Physical Chemistry C, 2007, 111, 6781-6788.	3.1	20
17	Ab initio study of the optical transitions on low-coordinated sites of an intermediate F center: The Fs+(OH)â^' center on MgO(100) surface. Solid State Ionics, 2007, 178, 173-178.	2.7	7
18	Comparison of the reduction of metal oxide surfaces: TiO2-anatase, TiO2-rutile and SnO2-rutile. Surface Science, 2005, 583, 107-117.	1.9	110

#	Article	IF	Citations
19	FS+ and FS+(OHâˆ') defect centers at the MgO(100) surface: cluster and periodic calculations. Surface Science, 2004, 549, 294-304.	1.9	24
20	Theoretical Study of the Acetonitrile Flip-Flop with the Electric Field Orientation: Adsorption on a Pt(111) Electrode Surface. Catalysis Letters, 2003, 91, 225-234.	2.6	20
21	Hartreeâ€"Fock study of the Si(l00) reconstruction. Computational and Theoretical Chemistry, 1998, 458, 171-189.	1.5	4
22	Theoretical Study of the TiO2 and MgO Surface Acidity and the Adsorption of Acids and Bases. Molecular Engineering, 1997, 7, 245-261.	0.2	19
23	Ab initio periodic pseudopotential Hartree-Fock calculations of O2 dissociation on perfect Si(100) surface. Journal of Molecular Catalysis A, 1997, 119, 185-193.	4.8	7
24	Theoretical Study of the TiO2 and MgO Surface Acidity and the Adsorption of Acids and Bases. Topics in Molecular Organization and Engineering, 1997, , 245-261.	0.1	2
25	A theoretical analysis of NH3 adsorption on TiO2. Surface Science, 1996, 365, 649-661.	1.9	75
26	A theoretical study of CO2 adsorption on TiO2. Computational and Theoretical Chemistry, 1996, 371, 219-235.	1.5	76