Xavier Aparicio-AnglÃ¨s

List of Publications by Year
in descending order

16 papers	291 citations	840776 11 h-index	940533 16 g-index
17 all docs	17 docs citations	17 times ranked	480 citing authors

#	Article	IF	Citations
1	Combined density functional theory and molecular dynamics study of Sm_{0.75}A_{0.25}Co_{1â^’x}Mn_xO_{2.88} (A = Ca, Sr;) Tj ETQq1 1 0.784314 rgB Chemical Physics, 2020, 22, 692-699.	2.8	10
2	Computational study of the mixed B-site perovskite SmB_xCo_{1â^’x}O_{3â^’d} (B = Mn, Fe, Ni, Cu) for next generation solid oxide fuel cell cathodes. Physical Chemistry Chemical Physics, 2019, 21, 9407-9418.	2.8	20
3	CO₂ and H₂ Adsorption and Reaction at Ni_{<i>n</i>}/YSZ(111) Interfaces: A Density Functional Theory Study. Journal of Physical Chemistry C, 2018, 122, 19463-19472.	3.1	15
4	Modeling of complex interfaces: Gadoliniumâ€doped ceria in contact with yttriaâ€stabilized zirconia. Journal of the American Ceramic Society, 2017, 100, 3329-3339.	3.8	9
5	A computational study of the electronic properties, ionic conduction, and thermal expansion of Sm_{1â^’x}A_xCoO₃and Sm_{1â^’x}A_xCoO_{3â^’x/2}(A = Ba²⁺, Ca²⁺,) Tj ETQq1 1 0.784314 rgBT /O Chemical Physics, 2017, 19, 13960-13969.	2.8	14
6	Counterintuitive Adsorption of [PW₁₁O₃₉]^{7â€“} on Au(100). Inorganic Chemistry, 2017, 56, 3961-3969.	4.0	18
7	Publisherâ€™s Note: â€œAb initio study of vacancy formation in cubic LaMnO3 and SmCoO3 as cathode materials in solid oxide fuel cellsâ€•[J. Chem. Phys. 145, 014703 (2016)]. Journal of Chemical Physics, 2016, 145, 199901.	3.0	2
8	A DFT+U study of the structural, electronic, magnetic, and mechanical properties of cubic and orthorhombic SmCoO3. Journal of Chemical Physics, 2016, 145, 224704.	3.0	15
9	Ab initio study of vacancy formation in cubic LaMnO3 and SmCoO3 as cathode materials in solid oxide fuel cells. Journal of Chemical Physics, 2016, 145, 014703.	3.0	25
10	Gadolinium-Vacancy Clusters in the (111) Surface of Gadolinium-Doped Ceria: A Density Functional Theory Study. Chemistry of Materials, 2015, 27, 7910-7917.	6.7	26
11	Endohedral Metallofullerenes Containing Lanthanides: A Robust Yet Simple Computational Approach. Journal of Physical Chemistry C, 2013, 117, 12916-12921.	3.1	15
12	Electronic structure of IPR and non-IPR endohedral metallofullerenes: Connecting orbital and topological rules. Comptes Rendus Chimie, 2012, 15, 152-158.	0.5	11
13	Polyoxometalates adsorbed on metallic surfaces: immediate reduction of [SiW12O40]4â^’ on Ag(100). Chemical Science, 2012, 3, 2020.	7.4	32
14	Towards the computational modelling of polyoxoanions on metal surfaces: IR spectrum characterisation of [SiW12O40]4â^’ on Ag(111). Physical Chemistry Chemical Physics, 2011, 13, 15143.	2.8	21
15	Theoretical view on the origin and implications of structural distortions in polyoxometalates. Physics Procedia, 2010, 8, 94-103.	1.2	8
16	Structural and Electrochemical Property Correlations of Metallic Nitride Endohedral Metallofullerenes. Journal of Physical Chemistry C, 2010, 114, 13003-13009.	3.1	48