Chiara Ricca

List of Publications by Year
in descending order

15	323	1163117 8	940533 16
papers	citations	h-index	g-index

16	16	16	499
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A comprehensive DFT investigation of bulk and low-index surfaces of ZrO₂polymorphs. Journal of Computational Chemistry, 2015, 36, 9-21.	3.3	61
2	Self-consistent <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>DFT</mml:mi><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:m study of oxygen vacancies in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></m Physical Review Research, 2020, 2, .	3.6	50
3	B,Nâ€Codoped graphene as catalyst for the oxygen reduction reaction: Insights from periodic and cluster DFT calculations. Journal of Computational Chemistry, 2018, 39, 637-647.	3.3	39
4	Self-consistent site-dependent DFT+ <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>U</mml:mi></mml:math> study of stoichiometric and defective <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SrMnO</mml:mi><mml:mn>3</mml:mn></mml:msub></ Physical Review B, 2019, 99, .	3.2	39
5	Oxidation of Ethylbenzene to Acetophenone with N-Doped Graphene: Insight from Theory. Journal of Physical Chemistry C, 2014, 118, 12275-12284.	3.1	35
6	Revealing the properties of the cubic ZrO2 (111) surface by periodic DFT calculations: reducibility and stabilization through doping with aliovalent Y2O3. RSC Advances, 2015, 5, 13941-13951.	3.6	22
7	Conduction Mechanisms in Oxideâ€“Carbonate Electrolytes for SOFC: Highlighting the Role of the Interface from First-Principles Modeling. Journal of Physical Chemistry C, 2018, 122, 10067-10077.	3.1	22
8	Mixed lithium-sodium (LiNaCO3) and lithium-potassium (LiKCO3) carbonates for low temperature electrochemical applications: Structure, electronic properties and surface reconstruction from ab-initio calculations. Surface Science, 2016, 647, 66-77.	1.9	18
9	Importance of surface oxygen vacancies for ultrafast hot carrier relaxation and transport in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>Cu</mml:mi><mml:mn>2</mml:mn></mml:msub></m O. Physical Review Research, 2021, 3, .	3.6	9
10	Defect Formation and Diffusion on the (001) Surface of LiKCO3 for Fuel Cell Applications: Insight from Hybrid DFT. Journal of Physical Chemistry C, 2016, 120, 12941-12951.	3.1	7
11	Modeling composite electrolytes for low-temperature solid oxide fuel cell application: structural, vibrational and electronic features of carbonateâ€“oxide interfaces. Journal of Materials Chemistry A, 2016, 4, 17473-17482.	10.3	6
12	Local polarization in oxygen-deficient LaMnO3 induced by charge localization in the Jahn-Teller distorted structure. Physical Review Research, 2020, 2, .	3.6	5
13	On the Stability Issues of TiO₂-Based Composites in View of Fuel Cell Application: A Combined Experimental and Theoretical Investigation. Journal of Physical Chemistry C, 2019, 123, 12573-12582.	3.1	3
14	Ferroelectricity promoted by cation/anion divacancies in SrMnO₃. Journal of Materials Chemistry C, 2021, 9, 13321-13330.	5.5	3
15	Photochemical anisotropy and direction-dependent optical absorption in semiconductors. Journal of Chemical Physics, 2022, 156, 154703.	3.0	1