

# Riccarda Caputo

## List of Publications by Year in descending order

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33  
papers

8,103  
citations

430442

18  
h-index

377514

34  
g-index

37  
all docs

37  
docs citations

37  
times ranked

10541  
citing authors

#	ARTICLE	IF	CITATIONS
1	Crystal Structure Prediction and Dehydrogenation Mechanism of $\text{LiMg}(\text{BH}_4)_3(\text{NH}_3)_2$ . Journal of Physical Chemistry C, 2021, 125, 10235-10242.	1.5	4
2	First-Principles Crystal Structure Prediction of Cu(I)-TCNQ Polymorphs. Journal of Physical Chemistry C, 2020, 124, 70-82.	1.5	7
3	Can lithium form phases with molybdenum?. Journal of Solid State Chemistry, 2019, 271, 230-238.	1.4	4
4	Topochemical Path in High Lithiation of $\text{MoS}_2$ . Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2019, 645, 309-316.	0.6	3
5	Allotropes of tellurium from first-principles crystal structure prediction calculations under pressure. RSC Advances, 2018, 8, 39650-39656.	1.7	9
6	Colloidal Bismuth Nanocrystals as a Model Anode Material for Rechargeable Mg-Ion Batteries: Atomistic and Mesoscale Insights. ACS Nano, 2018, 12, 8297-8307.	7.3	61
7	An Insight into Sodiation of Antimony from First-Principles Crystal Structure Prediction. Journal of Electronic Materials, 2016, 45, 999-1010.	1.0	17
8	Frontispiece: Seamless Rim-Functionalization of h-BN with Silica-Experiment and Theoretical Modeling. Chemistry - A European Journal, 2015, 21, n/a-n/a.	1.7	0
9	A theoretical and experimental study of the crystal structure of $\text{H}_2\text{V}_3\text{O}_8$ . RSC Advances, 2015, 5, 106543-106550.	1.7	17
10	Nanocrystals of Cesium Lead Halide Perovskites ( $\text{CsPbX}_3$ , X = Cl, Br, and I): Novel Optoelectronic Materials Showing Bright Emission with Wide Color Gamut. Nano Letters, 2015, 15, 3692-3696.	4.5	6,814
11	Seamless Rim-Functionalization of h-BN with Silica-Experiment and Theoretical Modeling. Chemistry - A European Journal, 2015, 21, 7662-7667.	1.7	2
12	A General Synthesis Strategy for Monodisperse Metallic and Metalloid Nanoparticles (In, Ga, Bi, Sb, Zn). Tj ETQqO O O rgBT /Overlock 10 635-647.	3.2	99
13	Monodisperse Colloidal Gallium Nanoparticles: Synthesis, Low Temperature Crystallization, Surface Plasmon Resonance and Li-Ion Storage. Journal of the American Chemical Society, 2014, 136, 12422-12430.	6.6	133
14	Precision synthesis of colloidal inorganic nanocrystals using metal and metalloid amides. Nanoscale, 2013, 5, 8398.	2.8	42
15	Ab initio crystal structure prediction by combining symmetry analysis representations and total energy calculations. An insight into the structure of $\text{Mg}(\text{BH}_4)_2$ . Physical Chemistry Chemical Physics, 2013, 15, 1471-1480.	1.3	13
16	Tailoring Two Polymorphs of $\text{LiFePO}_4$ by Efficient Microwave-Assisted Synthesis: A Combined Experimental and Theoretical Study. Chemistry of Materials, 2013, 25, 3399-3407.	3.2	40
17	Exploring the structure-composition phase space of lithium borocarbide, $\text{Li}_x\text{BC}$ for $x \approx 1$ . RSC Advances, 2013, 3, 10230.	1.7	4
18	Lithium Dihydroborate: First-Principles Structure Prediction of $\text{LiBH}_2$ . Inorganic Chemistry, 2012, 51, 9757-9765.	1.9	13

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19	Experimental Evidence of Na <sub>2</sub> [B <sub>12</sub> H <sub>12</sub> ] and Na Formation in the Desorption Pathway of the 2NaBH <sub>4</sub> +MgH <sub>2</sub> System. Journal of Physical Chemistry C, 2011, 115, 16664-16671.	1.5	46
20	A multifaceted approach to hydrogen storage. Physical Chemistry Chemical Physics, 2011, 13, 16955.	1.3	64
21	Ab-initio crystal structure prediction. A case study: NaBH <sub>4</sub> . Journal of Solid State Chemistry, 2011, 184, 1622-1630.	1.4	21
22	Stability and Decomposition of NaBH <sub>4</sub> . Journal of Physical Chemistry C, 2010, 114, 7173-7177.	1.5	174
23	Room-Temperature Synthesis of Nickel Borides via Decomposition of NaBH <sub>4</sub> Promoted by Nickel Bromide. Inorganic Chemistry, 2010, 49, 8756-8762.	1.9	21
24	Can Na <sub>2</sub> [B <sub>12</sub> H <sub>12</sub> ] be a decomposition product of NaBH <sub>4</sub> ?. Physical Chemistry Chemical Physics, 2010, 12, 15093.	1.3	49
25	First-Principles Determination of the Ground-State Structure of $\text{LiBH}_4$ . Physical Review Letters, 2010, 104, 215501.	2.9	45
26	First-principles study of the paths of the decomposition reaction of LiBH <sub>4</sub> . Molecular Physics, 2010, 108, 1263-1276.	0.8	17
27	First-principles determination of the ground-state structure of Mg(BH <sub>4</sub> ) <sub>2</sub> . Chemical Physics Letters, 2009, 480, 203-209.	1.2	38
28	Complex Hydrides with (BH <sub>4</sub> ) <sup>-</sup> and (NH <sub>2</sub> ) <sup>-</sup> Anions as New Lithium Fast-Ion Conductors. Journal of the American Chemical Society, 2009, 131, 16389-16391.	6.6	183
29	First principles study of $\pm$ -boron: can the B <sub>12</sub> cage host hetero-atoms?. Molecular Physics, 2009, 107, 1831-1842.	0.8	16
30	Phenol near Ni(111), Ni(110), and Ni(221) surfaces in a vertical ring geometry: A density functional study of the oxygen-surface bonding and O-H cleavage. Physical Review B, 2007, 75, .	1.1	31
31	Alkanethiol headgroup on metal (111)-surfaces: general features of the adsorption onto group 10 and 11 transition metals. Journal of Physics Condensed Matter, 2007, 19, 176004.	0.7	5
32	Adsorption of Benzene on Coinage Metals: A Theoretical Analysis Using Wavefunction-Based Methods. Journal of Physical Chemistry A, 2007, 111, 12778-12784.	1.1	38
33	Where do the H atoms reside in PdH <sub>x</sub> systems?. Molecular Physics, 2003, 101, 1781-1787.	0.8	71