## Claudia Caddeo

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

32	723	15	<b>26</b>
papers	citations	h-index	g-index
33 ext. papers	858 ext. citations	<b>6.1</b> avg, IF	4.32 L-index

#	Paper	IF	Citations
32	Theoretical insight on PTB7:PC71BM, PTB7-th:PC71BM and Si-PCPDTBT:PC71BM interactions governing blend nanoscale morphology for efficient solar cells. <i>Nano Energy</i> , <b>2021</b> , 82, 105708	17.1	3
31	Fundamentals of tin iodide perovskites: a promising route to highly efficient, lead-free solar cells. Journal of Materials Chemistry A, <b>2021</b> , 9, 11812-11826	13	12
30	Direct Correlation of Nanoscale Morphology and Device Performance to Study Photocurrent Generation in Donor-Enriched Phases of Polymer Solar Cells. <i>ACS Applied Materials &amp; Description</i> , 2020, 12, 28404-28415	9.5	3
29	Dielectric function of hybrid perovskites at finite temperature investigated by classical molecular dynamics. <i>Journal of Chemical Physics</i> , <b>2020</b> , 152, 104705	3.9	5
28	Ag/In lead-free double perovskites. <i>EcoMat</i> , <b>2020</b> , 2, e12017	9.4	12
27	The dominant role of surfaces in the hysteretic behavior of hybrid perovskites. <i>Nano Energy</i> , <b>2020</b> , 67, 104162	17.1	12
26	Donuts and Spin Vortices at the Fermi Surfaces of Hybrid Lead-Iodide CH3NH3PbI3 Perovskites. Journal of Physical Chemistry C, <b>2019</b> , 123, 6753-6762	3.8	2
25	Photoacoustic Sensing of Trapped Fluids in Nanoporous Thin Films: Device Engineering and Sensing Scheme. <i>ACS Applied Materials &amp; Device Engineering and Sensing Scheme</i> . <i>ACS Applied Materials &amp; Device Engineering and Sensing Scheme</i> . <i>ACS Applied Materials &amp; Device Engineering and Sensing Scheme</i> .	9.5	16
24	Hydrophilicity and Water Contact Angle on Methylammonium Lead Iodide. <i>Advanced Materials Interfaces</i> , <b>2018</b> , 6, 1801173	4.6	13
23	Development of a Classical Interatomic Potential for MAPbBr3. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 3724-3733	3.8	19
22	Thermal boundary resistance from transient nanocalorimetry: A multiscale modeling approach. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	15
21	Bottom-Up Mechanical Nanometrology of Granular Ag Nanoparticles Thin Films. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 22434-22441	3.8	23
20	Collective Molecular Mechanisms in the CHNHPbI Dissolution by Liquid Water. ACS Nano, 2017, 11, 918	83 <del>19</del> 61 <del>/</del> 90	0 49
19	Linking morphology to thermal conductivity in PEDOT: an atomistic investigation. <i>Journal Physics D: Applied Physics</i> , <b>2017</b> , 50, 494002	3	13
18	Photoluminescence, optical gain, and lasing threshold in CH3NH3PbI3 methylammonium lead-halide perovskites obtained by ab initio calculations. <i>Journal of Materials Chemistry C</i> , <b>2017</b> , 5, 127	758-127	768
17	Modeling hybrid perovskites by molecular dynamics. <i>Journal of Physics Condensed Matter</i> , <b>2017</b> , 29, 04	3008	45
16	Bulk Structural and Electronic Properties at the Density Functional Theory and Post-Density Functional Theory Level of Calculation <b>2017</b> , 43-86		

## LIST OF PUBLICATIONS

Structure and Thermodynamic Properties of Hybrid Perovskites by Classical Molecular Dynamics **2017**, 1-42

14	Thermally Activated Point Defect Diffusion in Methylammonium Lead Trihalide: Anisotropic and Ultrahigh Mobility of Iodine. <i>Journal of Physical Chemistry Letters</i> , <b>2016</b> , 7, 2356-61	6.4	93
13	Temperature Evolution of Methylammonium Trihalide Vibrations at the Atomic Scale. <i>Journal of Physical Chemistry Letters</i> , <b>2016</b> , 7, 529-35	6.4	66
12	Appealing Perspectives of Hybrid LeadIbdide Perovskites as Thermoelectric Materials. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 28472-28479	3.8	49
11	Low electron-polar optical phonon scattering as a fundamental aspect of carrier mobility in methylammonium lead halide CH3NH3PbI3 perovskites. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 15352-62	3.6	68
10	Tuning the thermal conductivity of methylammonium lead halide by the molecular substructure. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 24318-24	3.6	41
9	The study of polythiophene/water interfaces by sum-frequency generation spectroscopy and molecular dynamics simulations. <i>Journal of Materials Chemistry B</i> , <b>2015</b> , 3, 6429-6438	7.3	17
8	Pinpointing the Cause of Platinum Tipping on CdS Nanorods. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 22663-22668	3.8	2
7	Atomistic simulations of P(NDI2OD-T2) morphologies: from single chain to condensed phases. Journal of Physical Chemistry B, <b>2014</b> , 118, 12556-65	3.4	16
6	Atomistic Investigation of the Solubility of 3-Alkylthiophene Polymers in Tetrahydrofuran Solvent. <i>Macromolecules</i> , <b>2013</b> , 46, 8003-8008	5.5	26
5	Optoelectronic properties of (ZnO)60 isomers. <i>Physical Chemistry Chemical Physics</i> , <b>2012</b> , 14, 14293-8	3.6	13
4	Electronic Properties of Hybrid Zinc OxideDligothiophene Nanostructures. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 8174-8180	3.8	13
3	Poly(3-hexylthiophene) Adhesion on Zinc Oxide Nanoneedles. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 16833-16837	3.8	18
2	Understanding the Helical Wrapping of Poly(3-hexylthiophene) on Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , <b>2010</b> , 114, 21109-21113	3.8	52
1	Implementation of a <b>D</b> esign of Experiments Methodology for the Prediction of Phototransistor Degradation in a Space Environment. <i>IEEE Transactions on Nuclear Science</i> , <b>2009</b> , 56, 2465-2472	1.7	2