

Simon M-M Dubois

List of Publications by Year in descending order

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17
papers

830
citations

687363

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888059

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17
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1355
citing authors

#	ARTICLE	IF	CITATIONS
1	Organic-Inorganic Hybrid Interfaces for Spin Injection into Carbon Nanotubes and Graphene. <i>Advanced Quantum Technologies</i> , 2022, 5, .	3.9	1
2	Spin filtering by proximity effects at hybridized interfaces in spin-valves with 2D graphene barriers. <i>Nature Communications</i> , 2020, 11, 5670.	12.8	37
3	The <i>ONETEP</i> linear-scaling density functional theory program. <i>Journal of Chemical Physics</i> , 2020, 152, 174111.	3.0	94
4	Computational Atomistic Modeling in Carbon Flatland and Other 2D Nanomaterials. <i>Applied Sciences (Switzerland)</i> , 2020, 10, 1724.	2.5	2
5	Path to Overcome Material and Fundamental Obstacles in Spin Valves Based on MoS ₂ and Other Transition-Metal Dichalcogenides. <i>Physical Review Applied</i> , 2019, 12, .	3.8	13
6	Universal Spin Diffusion Length in Polycrystalline Graphene. <i>Nano Letters</i> , 2019, 19, 7418-7426.	9.1	15
7	Band-Structure Spin-Filtering in Vertical Spin Valves Based on Chemical Vapor Deposited WS ₂ . <i>ACS Nano</i> , 2019, 13, 14468-14476.	14.6	44
8	Insulator-to-Metallic Spin-Filtering in 2D-Magnetic Tunnel Junctions Based on Hexagonal Boron Nitride. <i>ACS Nano</i> , 2018, 12, 4712-4718.	14.6	88
9	The electronic and transport properties of two-dimensional conjugated polymer networks including disorder. <i>Nanoscale</i> , 2016, 8, 1642-1651.	5.6	19
10	Spin transport in hydrogenated graphene. <i>2D Materials</i> , 2015, 2, 022002.	4.4	81
11	Electronic transport calculations in the onetep code: Implementation and applications. <i>Computer Physics Communications</i> , 2015, 193, 78-88.	7.5	10
12	Anharmonic Infrared Spectroscopy through the Fourier Transform of Time Correlation Function Formalism in <i>ONETEP</i> . <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3321-3332.	5.3	20
13	Achievements of DFT for the Investigation of Graphene-Related Nanostructures. <i>Accounts of Chemical Research</i> , 2014, 47, 3292-3300.	15.6	15
14	Spin Filtering and Magneto-Resistive Effect at the Graphene/h-BN Ribbon Interface. <i>ACS Nano</i> , 2013, 7, 4578-4585.	14.6	21
15	Transport properties of graphene containing structural defects. <i>Physical Review B</i> , 2012, 86, .	3.2	157
16	Two-Dimensional Graphene with Structural Defects: Elastic Mean Free Path, Minimum Conductivity, and Anderson Transition. <i>Physical Review Letters</i> , 2011, 106, 046803.	7.8	105
17	Quantum Transport in Graphene Nanoribbons: Effects of Edge Reconstruction and Chemical Reactivity. <i>ACS Nano</i> , 2010, 4, 1971-1976.	14.6	108