

Sara Bonella's Publications

- M. Monteferrante, S. Bonella, G. Ciccotti "Quantum dynamical structure factor of liquid neon via a quasiclassical symmetrized method", J. Chem. Phys. 138, 054118 (2013) DOI: 10.1063/1.4789760
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- F. Sterpone, S. Bonella, S. Meloni "Early stage of the dehydrogenation of NaAlH₄ by ab initio rare events simulations", J. Phys. Chem. C, 19636-19643 (2012) DOI: 10.1021/jp3019588
- A. Poma, M. Monteferrante, S. Bonella, G. Ciccotti "The quantum free energy barrier for hydrogen vacancy diffusion in Na₃AlH₆", Phys. Chem. Chem. Phys., 14, 15458-15463 (2012) DOI: 10.1039/C2CP42536J
- W. Babiacyk, S. Bonella, G. Ciccotti, M. L. Coluccio, F. Gentile and E. Di Fabrizio "Silver self aggregation in a nanodevice for enhanced Raman spectroscopy: experiments vs simplified modeling via molecular dynamics", Nanoscale, 4, 2362-2371 (2012), DOI: 10.1039/c2nr30145h
- S. Bonella, S. Meloni and G. Ciccotti "Theory and methods for rare events", European Physical Journal B, 85, 97 (2012)
- M. Monteferrante, S. Bonella and G. Ciccotti "Linearized symmetrized quantum time correlation functions calculation via phase pre-averaging", Mol. Phys. 109, 3015-3027 (2011)
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