First-principle simulations of high pressure hydrogen

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First principle simulations results are crucial for the present understanding of the physics of hydrogen under extreme conditions of pressure and temperature. I will present a critical overview of those methods for Dense Hydrogen and describe some recent results [1]. In particular I will focus on recent developments to include nuclear quantum effects and how standard methods need to be modified accordingly. Finally I will illustrate predictions for the Metal-Insulator transition in liquid hydrogen[2,3,4] and for molecular and atomic crystalline hydrogen[5,6,7].

[1] J. M. McMahon, M.A. Morales, C. Pierleoni and D.M. Ceperley, "The properties of hydrogen and helium under extreme conditions", Rev. Mod. Phys. 84, 1607 (2012).
[2] M. A. Morales, C. Pierleoni, E Schwegler and D. M. Ceperley, "Evidence of a first order liquid-liquid transition in high pressure hydrogen from ab-initio simulations", PNAS 107, 12799 (2010).
[3] E. Liberatore, M. A. Morales, D. M. Ceperley and C. Pierleoni, "Free energy methods in Coupled Electron-Ion Monte Carlo", Mol. Phys. 109, 3029 (2011).
[4] M.A. Morales, J.M. McMahon, C. Pierleoni and D.M. Ceperley, "Nuclear Quantum Effects and Nonlocal Exchange-Correlation Functionals Applied to Liquid Hydrogen at High Pressure", Phys. Rev. Letts. 110, 065702 (2013).
[5] M.A. Morales, J.M. McMahon, C. Pierleoni and D.M. Ceperley, "Towards a predictive First-Principle Description of Solid Molecular Hydrogen with Density-Functional Theory", Phys Rev B 87, 184107 (2013).
[6] J. Chen, X.-Z. Li, Q. Zhang, M. I. J. Probert, C. J. Pickard, R. J. Needs, A. Michaelides, and E. Wang, "Quantum simulation of low-temperature metallic liquid hydrogen", Nature Communications 4, 2064 (2013).
[7] J.M. McMahon, M.A. MOrales, C. Pierleoni and D.M. Ceperley,"Atomic hydrogen: a ground-state fluid or a metallic solid?", submitted (2013).