"Recent progress in the electronic simulation by ab-initio molecular dynamics and quantum Monte Carlo forces"

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Abstract:

We describe recent progress for the simulation of realistic systems by a recently developed ab-initio molecular dynamics[1-3]. In this dynamics accurate forces are computed by advanced quantum Monte Carlo techniques, and by using a many-body wave function that has been extensively tested to give state of the art results for the description of the chemical bond, even in the strongly correlated regime. In high pressure hydrogen, we have carried out an extensive and systematic study by using this method with large simulation supercell containing up to 256 protons. We find that the molecular liquid phase is unexpectedly stable and the transition towards a fully atomic liquid phase occurs at much higher pressure than previously believed. The old standing problem of low temperature atomization is, therefore, still far from experimental reach. Finally we also describe recent progress in the simulation of liquid water at ambient conditions, that, we will show, is becoming feasible even within the present quantum Monte Carlo method.

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[2] S. Sorella and L. Capriotti, J. Chem. Phys. 133, 234111 (2010).
[3] G. Mazzola, S. Yunoki and S. Sorella, in press.