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Towards an hybrid representation in the KSDFT simulations at high temperature JEAN CLEROUIN, AUGUSTIN BLANCHET, MARC TORRENT, CEA, DAM, DIF 91297 Arpajon, France — Orbital-based Kohn-Sham resolution of density functional theory is now a very popular method to describe condensed matter systems. Low temperature disordered systems can be considered through the finite temperature extension of the method and combined with molecular dynamics (KSMD). At high temperature, however, this approach becomes prohibitively expensive due to the huge number of quasi-empty orbitals to consider. KSMD simulations are just unattainable beyond a few tens of eVs, and must be replaced by their semi-classical counterpart, namely the orbital-free molecular dynamics method (OFMD). Even if the transition from KSMD to OFMD is well documented, a continuous transition inside a unique frame would be desirable. Inspired by a recent work1 we have implemented in the Abinit code a scheme that substitutes high energy orbitals by plane waves allowing for a much smaller orbitals basis sets and thus much faster calculations at high temperatures while keeping the orbital based precision at low temperature. A rewriting of the Kubo-Greenwood conductivity should allow for a global formulation valid in all regimes of temperatures. We intend to apply this methods to the calculation of Jupiter's isentrope keeping the same level of precision and statistics between computations at the surface of Jupiter, mainly made of molecular hydrogen, and at the core of the planet with metallic hydrogen at few tens of Mbar. [1] Shen Zhang, Hongwei Wang, Wei Kang, Ping Zhang, and X. T. He. Physics of Plasmas, 23(4): 042707, April 2016.

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