Ab initio calculation of equation of state of crystalline molecular hydrogen with nuclear quantum effects at high pressures

Bystryi R G[1,2] **and Saitov I M**[1,2,3,@]

[1] National Research University Higher School of Economics, Myasnitskaya 20, Moscow 101000, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[3] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia

[@] saitovilnur@gmail.com

The metallization of crystalline hydrogen at high pressures has been theoretically investigated since 1935. In the original work [1], it is assumed that hydrogen molecules dissociate, forming a body-centered cubic lattice with one proton per unit cell. There are two suggested mechanisms of the formation of metallic solid hydrogen. The first mechanism is based on the prediction of [1] and is associated with the dissociation of hydrogen molecules with the formation of an atomic lattice. The second mechanism assumes that the metallization of the crystalline hydrogen is associated with overlapping of the conduction and valence bands and structural transformations, but the hydrogen crystal remains molecular. In this work we apply path integral molecular dynamics with the framework the density functional theory in order to study the influence of nuclear quantum effects (NQEs) and nonlocal exchange-correlation density functionals near metallization of crystalline molecular hydrogen. NQEs influence bond stability in hydrogen molecule and, therefore the pressure of metallization as it was in [2] for the similar phase transition in fluid hydrogen. The work is prepared within the framework of the HSE University Basic Research Program.

[1] Wigner E and Huntington H B 1935 *J. Chem. Phys.* **3** 764–770
[2] Morales M A, McMahon J M, Pierleoni C and Ceperley D M 2013 *Phys. Rev. Lett.* **110** 065702