Kinetics of plasma phase transition in dense fluid H_2: The analysis based on first-principles molecular dynamics

Fedorov I D[1,2,3] **and Stegailov V V**[1,2,3,@]

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

[@] stegailov.vv@phystech.edu

The transition of warm dense fluid hydrogen from an insulator to a conducting state at pressures of about 20-400 GPa and temperatures of 500-5000 K has been the subject of active scientific research over the past few decades. However, various experimental and theoretical methods do not provide consistent results. In this work, we propose a novel exciton dissociation mechanism for the transition of molecular fluid H_2 from molecular state to plasma. This mechanism is able to give a quantitative description of several experimental results as well as to resolve their discrepancies.
The quantitative results that support the proposed mechanism are based on first-principles molecular dynamics (FPMD) within the restricted open-shell Kohn-Sham (ROKS) method [1, 2]. We use ROKS to model dense hydrogen after thermal excitation to the first singlet excited state. The Wannier localization method has allowed us to analyze the exciton dynamics in this system. The ROKS model shows that a key mechanism of the transition is associated with the dissociation of electron-hole pairs, which allows explaining several stages of the transition of fluid H_2 from molecular state to plasma [3].

[1] Fedorov I D, Orekhov N D and Stegailov V V 2020 *Phys. Rev. B* **101** 100101
[2] Fedorov I D and Stegailov V V 2021 *JETP Letters* **113** 396–401
[3] Fedorov I D and Stegailov V V *ChemPhysChem* 10.1002/cphc.202200730