

EXCITON MECHANISM OF WARM DENSE MOLECULAR HYDROGEN METALLIZATION

Fedorov I.D.,^{*1,2} *Stegailov V.V.*^{1,2,3}

¹*MIPT, Dolgoprudny, Russia,* ²*JIHT RAS, Moscow, Russia,* ³*HSE,*

Moscow, Russia

**ilya.d.fedorov@phystech.edu*

Insulator-to-metal transition (IMT) in fluid warm dense hydrogen (WDH) is one of the unresolved problems of the last decades. There are a large number of experiments aimed at determining this transition, but they have a large number of disagreements.

This work is the result of a rethinking of theoretical works and a search for the cause of the disagreement between the results of theory and experiment. The first step was to study the applicability of the finite temperature density functional theory (FT DFT) under the conditions of the considered fluid transition [1]. The study of the dynamics of individual electronic excitations showed significantly longer times of electronic transitions than is suggested by FT DFT. The second step was to study the behavior and properties of such an excited electronic state [2], which showed the presence of a bound exciton state at certain temperatures, and the absence of this coupling with increasing temperature. The aim of this work is to obtain the P-T dependence of excitonic transitions and its relationship with experimental observations.

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 2. Fedorov I. D., Stegailov V. V. // *JETP Lett.* 2021. V. 113. No. 6. P. 396-401.