ФОРМИРОВАНИЕ И ДИНАМИКА ЭКСИТОНОВ В РАЗОГРЕТОМ ПЛОТНОМ МОЛЕКУЛЯРНОМ ФЛЮИДЕ АЗОТА В УСЛОВИЯХ ЭКСПЕРИМЕНТОВ ПО СВЕРХБЫСТРОМУ НАГРЕВУ

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Understanding the properties of molecular nitrogen N_2 at extreme conditions is the fundamental problem for atomistic theory and the important benchmark for the capabilities of first-principles molecular dynamics (FPMD) methods. In this work, we extend our previous results for dense molecular H_2 [1] and focus on the connection between the dynamics of ions and electronic excitations in warm dense N_2 [2]. The restricted open-shell Kohn-Sham (ROKS) method gives us the possibility to reach relevant time and length scales for FPMD modelling of an isolated exciton dynamics in warm dense N_2. Wannier localization sheds light on the corresponding mechanisms of covalent bond network rearrangements that stand behind polymerization kinetics. FPMD results suggest a concept of energy transfer from thermal energy of ions into the internal energy of polymeric structures that form in warm dense N_2 at extreme conditions. Our findings agree with the thermobaric conditions for the onset of absorption in the optical spectroscopy study of Jiang et al. [3].

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1. Fedorov I. D., Stegailov V. V., ChemPhysChem **24** e202200730 (2023)
2. Fedorov I. D., Stegailov V. V., J. Chem. Phys. **161** 154503 (2024)
3. Jiang S., Holtgrewe N., Lobanov S. S., Su F., Mahmood M. F., McWilliams R. S., Goncharov A. F., Nat. Comm. **9**, 2624 (2018)