THEORETICAL INVESTIGATION OF ELECTRONIC STRUCTURE OF MOLECULES

Moscow Institute of Physics and Technology (National Research University)

Degree or qualification is awarded: **PhD (Candidate of Science)**

Language of study: **English**
Mode of study: **full-time**
Duration: **4 years**
Availability of free education: **no**
Price: **375 000 RUB**

Programme webpage at the university website:
https://eng.mipt.ru/programs/theoretical-investigation-of-electronic-structure-of-molecules/

Programme curator: **Denis Ustyuzhaninov**
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Entry requirements:

- Master's degree / equivalent in a related field
- B2 level of English
- Good track record of publications related to the topic of the intended research
- Strong research proposal 1,500 - 3,500 words

Research supervisor:
Alexander Mitin
PhD, DSc

Supervisor's research interests:
Theoretical investigation of electronic structure of molecules by ab initio methods. Development of the new methods, numerical algorithms, and computer programs of ab initio methods.

Supervisor's specific requirements:

- Knowledge of the ab initio methods: Hartree-Fock, configuration interaction, coupled cluster, density functional.
- Experience with ab initio programs: Molpro, Gaussian, CFour, or similar.

Main publications:

- A.V. Mitin, Unusual chemical bonding in the beryllium dimer and its twelve vibrational levels, Chem. Phys. Lett., 2017, 682, 30 (2017).
- A.V. Mitin and C. Van Wüllen, Two-Component Relativistic Density Functional Calculations of the Dimers of the Halogens from Bromine through Element 117 Using Effective Core Potential and AllElectron Methods, J. Chem. Phys., 124, 064305 (2006).

- A.V. Mitin, J. Baker, P. Pulay, An Improved 6-31G* Basis Set for First-Row Transition Metals, J. Chem. Phys., 118, 7775 (2003).

Specializations within this programme