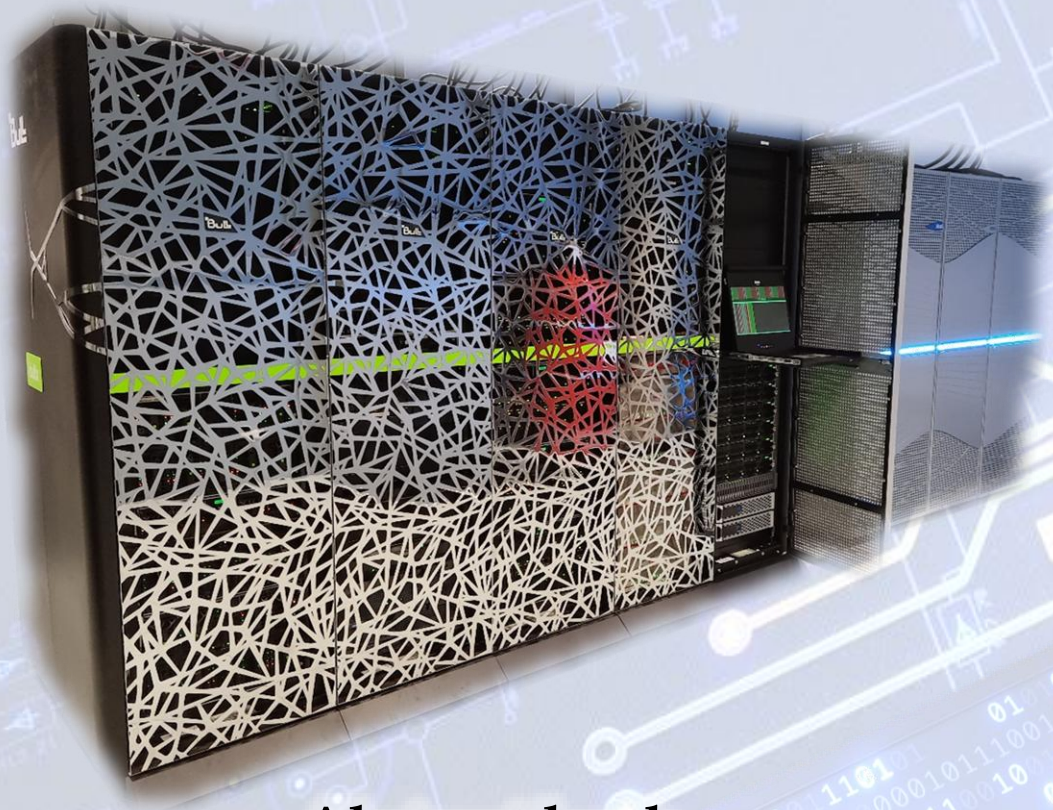
4TH EUROCC VILNIUS HACKATHON & WORKSHOP ON USING HPC



Abstract book

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Vilnius, Lithuania

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VILNIUS TECH

Lietuvos hidrometeorologijos tarnyba

Dynamics of excitation from excitons to polarons in molecular complexes

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A standard model of excitation in tightly coupled moelcular aggregate is the Frenkel exciton model. The main feature of the model is the emergence of collective coherent electronic excitations, which are delocalized due to resonant intermolecular couplings. Intramolecular vibrations introduce exciton decoherence and localization of the excitons, what is often denoted as self-trapping.

Harmonic model of molecular vibrations (Fig. 1) yields the Holstein model Hamiltonian, which has the bilinear form of the exciton-vibration interactions – the vibrational coordinate induces the excitation energy fluctuations. However, the exciton excited states are not thermalized states, so they are poor reference set of states, when coupling to vibrations is strong. Polaron transformation yields different set of states, which are equilibrated with respect to the static phonons, however they may poorly reflect dynamical effects. Partial polaron transformation [1] allows for fine tuning between the exciton and polaron models.

Choosing right reference states may yield rapidly converging equations of motion for the excitation dynamics. A closed new set of equations, based on the Nonlinear Exciton Equations [2] is derived for exciton-polaron dynamics. The equations allow for explicit n-particle quantum model for a exciton-vibrational systems.

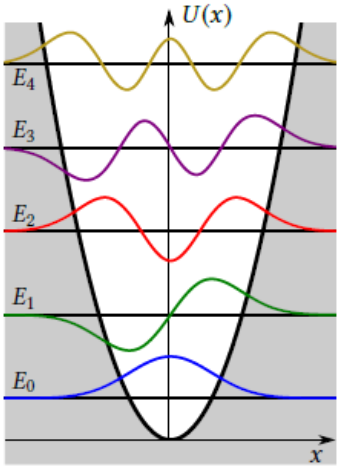

Fig. 1 harmonic model of molecular vibration: E0-E4 denote five lowest energy states of an oscillator, which would be included in five-particle quantum model.

REFERENCES

[1] Seogjoo J. Jang, Partially polaron-transformed quantum master equation for exciton and charge transport dynamics, *J. Chem. Phys.* 157, 104107 (2022).

[2] Vytautas Bubilaitis, Darius Abramavicius, Compact modeling of highly excited linear aggregates using generalized quantum particles, *Chem. Phys.* 588, 112445 (2025).