Applications are invited for a postdoctoral position in quantum molecular dynamics in the group of Prof. Irene Burghardt at Goethe University Frankfurt, in a collaborative project with Prof. Rocco Martinazzo, University of Milano. We aim to apply and further develop efficient quantum and quantum-classical multiconfigurational approaches using time-evolving Gaussian basis sets. Applications focus on multi-state exciton dynamics, transport, and time-resolved spectroscopies of functional molecular materials.

Requirements include a PhD in physics or theoretical chemistry, background in computational quantum dynamics, and experience in programming and scripting. Applicants are expected to bring strong motivation and creativity for theoretical, methodological, and numerical work. German language skills are not mandatory.

The two-year position is available from 1 May 2022 onwards, at a E13 TV-G-U (full time) funding level. Applications will be considered until the position is filled. Applicants should submit a CV, a brief statement of research interests, and the names of two referees, by e-mail to Prof. Irene Burghardt (burghardt@chemie.uni-frankfurt.de).

Relevant publications include:

R. Martinazzo and I. Burghardt, Local-in-time error in variational quantum dynamics, Phys. Rev. Lett. 124, 150601 (2020), https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.124.150601

D. Brey et al., Signatures of coherent vibronic exciton dynamics and conformational control in two-dimensional electronic spectroscopy of conjugated polymers, Faraday Discuss., in press (2022), https://doi.org/10.1039/D2FD00014H

F. Di Maiolo et al., Multi-layer Gaussian-based multi-configuration time-dependent Hartree (ML-GMCTDH) simulations of ultrafast charge separation in a donor-acceptor complex, J. Chem. Phys. 154, 144106 (2021), https://doi.org/10.1063/5.0046933

W. Koch et al., Two-layer Gaussian-based MCTDH study of the S1-S0 vibronic absorption spectrum of formaldehyde using multiplicative neural network potentials, J. Chem. Phys. 151, 064121 (2019), https://doi.org/10.1063/1.5113579

D. Picconi et al., Quantum dynamics and spectroscopy of dihalogens in solid matrices.II .Theoretical aspects and G-MCTDH simulations of time-resolved coherent Raman spectra of Schroedinger cat states of the embedded I2Kr18 cluster, J. Chem. Phys. 150, 064112 (2019), https://doi.org/10.1063/1.5082651

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