## Freie Universität Berlin - Fachbereich Physik - Institut für Theoretische Physik

The Clementi's group in the Physics Department at Freie Universität Berlin seeks a postdoctoral researcher to work on the development and application of coarse-graining methodologies to study macromolecular dynamics with machine learning and experimental data, integrative structural biology, and membrane protein modeling. Our group works on the definition and implementation of strategies to study complex biophysical processes on long timescales. We use data-driven methods for systematic coarse-graining of macromolecular systems, to bridge molecular and cellular scales. We work on a theoretical formulation to exploit the complementary information that can be obtained in simulation and experiment, to combine the approximate but high-resolution structural and dynamical information from computational models with the “exact” but lower resolution information available from experiments.

# Research assistant (postdoc) (m/f/d)

City: Berlin; Starting Date: At the earliest possible; Duration: limited to 31.12.2022; Renumeration: EG 13 TV-L FU; Reference number: WiMi_SFB1078_TPC7; Closing date: 01/02/21

### Working field

- Coupling of proton dynamics with large structural rearrangements in Phytochromes (WP1)
- Structural model of protein M of the Dengue virus and the West Nile Virus (WP2)

The project is part of the research consortium of the CRC 1078. The candidate will study global change in phythochromes. Using a multi-scale approach, we will combine this with atomistic MD and QM/MM simulations, in close collaboration with other projects of the SFB, to understand the coupling of long-time scale conformational changes with protonation states of the chromophore binding pocket.
We will proceed with the study of the dynamical and functional properties of protein M of DENV and WNV and its role in the proton transfer activity. As the atomistic structure of protein M is not known for any Flavivirus, nor its oligomerization state in DENV and WNV, the structural modelling will be the starting point of our project. In particular, the atomic structure and oligomerization state that will result from our modelling will be the starting point for the study of proton and cation permeation in these viroporins using atomistic MD and QM/MM simulations.

### Requirements

**Requirements: **
- Candidates must have a Ph.D. in Physics, Chemistry, Applied Mathematics, or related fields.

**Desirable: **
- Previous experience with macromolecular modeling and molecular dynamics simulations

- Excellent theoretical and practical experience with machine learning methods and the design of coarse-grain protein models is desirable.
- English language fluent, spoken and written.

**Application**

All applications (including a short cover letter outlining your background, a detailed CV including possibly some references, and all relevant certificates) quoting the **reference code** should be directed **no later than February 1st, 2021** preferably electronically in one PDF-file to: Mrs. Prof. Dr. Cecilia Clementi: **ammonlassen@physik.fu-berlin.de** or postal to

Freie Universität Berlin
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Institut für Theoretische Physik
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With an electronic application, you acknowledge that FU Berlin saves and processes your data. FU Berlin cannot guarantee the security of your personal data if you send your application over an unencrypted connection.

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More information at https://stellenticket.de/88100/BUA/
Offer visible until 01/02/21