



## Postdoctoral Researcher Position - Theoretical and Computational Chemistry

Applications are invited for a postdoctoral position in the group of Prof. William Glover at NYU Shanghai to develop polarizable embedding methodology to simulate photoexcited charge-transfer (CT) dynamics in multichromophoric systems. The specifics of the project are to achieve linear scaling in the integral-exact direct reaction field method, developed by our group in [doi.org/10.26434/chemrxiv-2022-15cjt](https://doi.org/10.26434/chemrxiv-2022-15cjt) and [doi.org/10.26434/chemrxiv-2022-j8rgj](https://doi.org/10.26434/chemrxiv-2022-j8rgj). The methodology will be applied to address the origins of high efficiency and unidirectionality in the primary CT reactions of the purple bacteria reaction center ([doi.org/10.26434/chemrxiv-2022-mkfzd](https://doi.org/10.26434/chemrxiv-2022-mkfzd)). Much of the development utilizes Graphical Processing Unit (GPU)-based quantum chemistry code. The project is funded by the National Natural Science Foundation of China. More details can be found at [wp.nyu.edu/glover](http://wp.nyu.edu/glover).

Research at NYU Shanghai is supported by the Center for Computational Chemistry, a research institute operated jointly by NYU, NYU Shanghai, and East China Normal University (ECNU). The center has a core group of faculty members who are conducting frontier research in various fields of theoretical/computational chemistry, biology, and materials science. More details can be found at [research.shanghai.nyu.edu/chemistry](http://research.shanghai.nyu.edu/chemistry).

Candidates should have the following qualifications:

- Ph.D. in Chemistry or Physics or related fields by the position start date
- Experience with molecular/quantum dynamics
- Experience developing electronic structure code
- Strong command of written and spoken English

Competitive candidates will also have expertise in one or more of the following: polarizable embedding, excited-state electronic structure methods, analytical gradient theory, diabaticization methods.

The position is available immediately or upon agreement. Benefits and salary are competitive. The position term is for 12 months initially, with possibility of extension.

Applications will be reviewed until the position is filled. To be considered, applicants should submit a cover letter with a brief description of research accomplishments and interests, a curriculum vitae with a list of publications, and the names and contact information of at least two references by e-mail to [william.glover@nyu.edu](mailto:william.glover@nyu.edu)

### *About NYU Shanghai:*

NYU Shanghai is the third degree-granting campus within New York University's global network. It is the first higher education joint venture in China authorized to grant degrees that are accredited in the U.S. as well as in China. All teaching is conducted in English. A research university with liberal arts and science at its core, it resides in one of the world's great cities with a vibrant intellectual community. NYU Shanghai recruits scholars of the highest caliber who are committed to NYU's global vision of transformative teaching and innovative research and who embody the global society in which we live.

NYU's global network includes degree-granting campuses in New York, Shanghai, and Abu Dhabi, complemented by twelve additional academic centers across five continents. Faculty and students circulate within the network in pursuit of common research interests and cross-cultural, interdisciplinary endeavors, both local and global.

NYU Shanghai is an equal opportunity employer committed to equity, diversity and social inclusion. We strongly encourage applications from individual who are under-represented in the profession, across color, creed, race, ethnic and national origin, physical ability, and gender and sexual identity. NYU Shanghai affirms the value of differing perspectives on the world as we strive to build the strongest possible university with the widest reach.

EOE/AA/Minorities/Females/Vet/Disabled/Sexual Orientation/Gender Identity Employer