NATIONAL SUPERCOMPUTING MISSION

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Cytoplasmic membrane

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Applications are invited from Indian natic / Research Associate" in the NSM-spons and Engine for Simulations of Photoindu

Project description: The project involves development of a comprehensive toolkit for computer simulations of photo-induced phenomena based on the combination of two excited state dynamics approaches: *ab initio* techniques (based on TDDFT), and open quantum system approaches (based on simple models). Target applications shall include solar energy conversion (photovoltaics, water-splitting catalysts, solar fuels, etc.), opto-electronic materials, photochemistry and photobiology.



Duration: Initially 12 months (up to two years with satisfactory performance).

Last date for applications: The selection will commence on 10 January 2021, but the call will remain open until suitable candidates are found.

Essential Qualifications: Ph.D in Computational Chemistry/Computational Quantum Physics/Theoretical Condensed Matter Physics with good academic record.

Desirable Qualifications: Experience with DFT/TDDFT codes, classical / *ab initio* MD, excited state dynamics (surface hopping / Ehrenfest dynamics), open quantum systems, energy transport, photo-physics.

Salary: In the range of Rs. 40,000 - 90,000 p.m. + HRA (16%), depending on experience.

How to Apply: Applications containing an (i) cover letter, (ii) updated CV with name and address of 2 referees, (iii) a 1-page writeup on their PhD thesis should be sent by e-mail **ONLY** to <u>vardha@iiserb.ac.in</u> on or before 10th January, 2021. Shortlisted candidates will be called for an interview in Bhopal (no TA shall be provided).

For more details and context see the homepage of **Dr. Varadharajan Srinivasan (ab** initio methods) and **Dr. Sebastian Wüster (open quantum systems)**.