Atoms and Computers

Prof. Michele Parrinello

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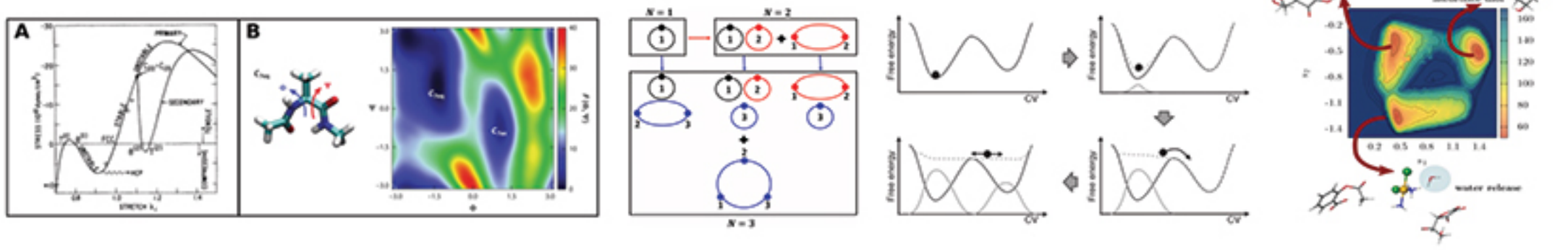

- Professor M. Parrinello who started his career in computational science with Prof. Anees Rahman (who is originally from Hyderabad) at Argonne National Laboratory has given many new simulation techniques to chemists, physicists and scientists working in biology. Among these are the Parrinello- Rahman Variable Shape Simulation Method, Car-Parrinello Molecular Dynamics (CPMD), Metadynamics and Variational Enhanced Sampling (VES).

  He has been the recipient of many awards: Schroedinger Medal, Sidney Fernbach Award, Hirschfelder Prize, Enrico Fermi Prize, Berni J. Alder CECAM Prize, Rahman Prize (with R. Car), Boys-Rahman Prize, Dreyfus Prize in the Chemical Sciences, ISQBP Award in Computational Biology, etc.

- The rapid development of computer technology and of efficient algorithms has had a deep impact on science. Of particular significance has been the emergence of realistic atomistic simulations. These calculations provide precious insight, replace difficult experiments, predict new phenomenon, and are also used to help build the computers of the future that will in turn be used to simulate ever more complex phenomena. We shall illustrate the power of this approach with a number of examples taken from different branches of science. Yet in spite of remarkable progress much remains to be done to widen the scope of atomistic simulations, especially in the fields of nanotechnology and biosciences. This requires new technical as well as conceptual tools in order to describe the complexity of the phenomena that contemporary science has to tackle. Avenues of progress will be presented.

DATE
February 17, 2020

TIME
4:00 p.m.

VENUE
MRC Auditorium

ALL ARE WELCOME ○ Tea/Coffee at 5:00 pm