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"First-Principles Based Design of New Materials for Nanotechnology, with applications to CO_2 and H_2 storage, Fuel Cells, solar cells, and Li batteries"

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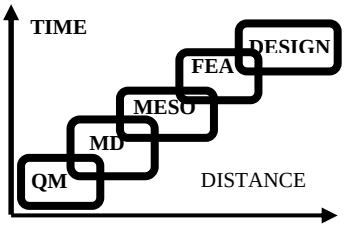

Advances in theoretical and computational chemistry are making it practical to consider fully first principles (de novo) predictions of important systems and processes in the Chemical, Biological, and Materials Sciences. Our approach to applying first principles to such systems is to build a hierarchy of models each based on the results of more fundamental methods but coarsened to make practical the consideration of much larger length and time scales. Connecting this hierarchy back to quantum mechanics enables the application of first principles to the coarse levels essential for practical simulations of complex systems.

We will highlight some recent advances in methodology and will illustrate them with recent applications related to Nanotechnology, Renewable Energy, Fuel Cells, Batteries, and Water Sustainability, selected from

- CO2 and H2 storage in MOF, COF, and ZIF reticular systems
- Oxygen reduction reaction (ORR) catalysts with decreased Pt for the fuel cell cathode
- CIGS Solar Cells
- New materials for Li batteries