



12th July 2018, 15:00 s.t.

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AG Molecular Quantum Dynamics

Application of Metadynamics to the Study of the Phenylisocyanate (PHI) and Cyclohexanol (CH-ol) Reaction.

Polymerization reactions are used to manufacture materials having a wide range of properties. However, despite its significance, little is known about the molecular details of the polymerization reactions. In general, theoretical calculations of the free energy of activation are rather demanding compared to experimental measurements. The state of affairs for the alcoholysis reaction of the isocyanate group forming the urethane bond in long polymers chains will be presented. Until now no dynamic study of such systems has been performed, so it will be discussed the application of metadynamics for the exploration of the free energy surface and the calculation of the reaction path. The importance of choosing an appropriate set of collective variables to describe the free energy surface will be highlighted.

Talk: English

Slides: English

Location: Institute of Physics, Albert-Einstein-Str. 24, HS 1