ICCRAM Scientific Conference Series on
Advanced Materials, Critical Raw Materials
and Industrial Technologies

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REACTION PATH SAMPLING USING RARE EVENT SIMULATION

Dr. Titus Van Erp

Norwegian University of Science and Technology (NTNU)

Profesor Van Erp is a World-leading expert in advanced simulation methods, mainly in path sampling simulation techniques for the study of rare events. Among the methods he developed are Transition Interface Sampling (TIS), Partial Path TIS (PPTIS), Replica Exchange TIS (RETIS), and QuanTIS.
Van Erp got recently **a 1.5 million euro grant by the Research Council of Norway to develop this idea further.**
Prof. Van Erp has also made important contributions to advanced **Monte Carlo methods** for the study of the adsorption of multi-component gas mixture in zeolite and als specific techniques for the adsorption of chiral compounds. For this work van Erp was selected for the **ESEP ExxonMobil young-researcher prize** that rewards a young researcher who made major contributions to the field of petrochemical research.
Van Erp has brought out about 50 publications and received several grants like the **Marie-Curie individual fellowship.**

Salón de Actos de la Facultad de Ciencias
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12.00 horas

Molecular simulation has become indispensable tool to gain insight in chemical and biological processes. Using either classical force fields or density functional theory based molecular dynamics (MD) one can, in principle, model reactive events on a reasonable realistic level. However, in contrast to most experiments where rate constants are obtained by measuring macroscopic quantities of reactants and products over a long time (seconds), MD simulations have to obtain good statistics with much smaller systems in the accessible time range of nanoseconds–microseconds. Therefore, the computation of rate constants with straightforward MD becomes inefficient when the process of interest has to overcome a high activation barrier because the probability to observe a reactive event on this time- and system-scale decreases exponentially with the barrier height. The transition interface sampling (TIS) technique allows large free energy barriers to be overcome within reasonable simulation time. Still, the method does not impose an artificial driving force, but it surmounts the timescale problem by a Monte Carlo sampling of true (MD based) dynamical pathways. In this talk I will discuss the method and some of its applications. In addition, I will discuss some recent method developments such as Replica Exchange TIS (RETIS) and the QuanTIS method. The later can be viewed as a dynamical analogue of the famous QM/MM method in which quantum mechanics and classical force fields are connected in time rather than in space.

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