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CV/ biography

Normand Mousseau is professor of physics at Université de Montréal and academic director of the Trottier Energy Institute. He holds a Ph.D. in physics from Michigan State University and he pursued post-doctoral studies at the University of Oxford and Université de Montréal. He was professor at Ohio University before moving to his current position in 2001. His work focuses on the atomistic kinetics of complex materials and biomolecules, with more than 180 scientific articles. Over the years, he has developed numerous simulation methods, such as the activation-relaxation technique (ARTn) and kinetic ART, for exploring the energy landscape of these materials and accessing experimental time scales. His codes are used by tens of groups from around the world.

He intervenes regularly on energy, climate and questions regarding science and society and has authors numerous books on these topics. In 2013, he co-chaired Quebec's Commission on energy issues. His latest book « Pandémie. Quand la raison tombe malade» was published by Éditions du Boréal in Novembre 2020.

Understanding the kinetics of formation of nanostructures through energy surfaces

Atoms move and assemble following local rules that can be understood, in a collective sense, as a walk of a system on an energy surface that describes its physics. While this concept is a useful way to approach often complex atomistic kinetics, this high-dimensional construction remains challenging to fully picture and characterize quantitatively. In recent years, many tools have been developed to explore, describe and classify the energy landscape of complex materials. For example, using various exploration methods, such as the activation and relaxation technique (ART nouveau) — a very efficient open-ended transition-point search method— and kinetic ART — an off-lattice kinetic Monte Carlo algorithm with on-the-fly catalog building, we have attempted to conduct exhaustive sampling in various systems, ranging from crystalline metals with amorphous semiconductors. The results of these studies allow us to better understand the diversity of diffusion mechanisms .In this presentation, I will rapidly provide an overview of these and other numerical and theoretical approaches developed to characterize the energy landscape of complex systems and nanostructures.

Building on our recent work that explains the correlations between the diffusion barrier and the prefactor, a correlation called “compensation law” or “Meyer-Neldel law”, I will also discuss why it is necessary to go beyond the energy mapping to include entropic effects to provide a more accurate description of the atomistic kinetics of nanostructured materials.

Keywords: Atomistic kinetics ; energy surface ; activation-relaxation technique ; kinetic ART; kinetic Monte Carlo; Meyer-Neldel Law; formation of nanostructures; disordered materials