CIC biomaGUNE
Biomaterialetako Ikerkuntza Kooperatiboko Zentroa
Center for Cooperative Research in Biomaterials

SEMINAR

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Host: Dr. Ivan Coluzza

Machine learning in atomistic simulations: from reaction pathways to phase diagrams

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Atomistic computer simulations of processes occurring in condensed matter systems are challenging for several distinct but related reasons. For large systems, the accurate calculation of energies and forces needed in molecular dynamics simulations may be computationally demanding, particularly if electronic structure calculations are used for this purpose. Other difficulties arising in the dynamical simulation of condensed matter processes consist in detecting local structures characteristic for stable or metastable phases and in identifying important degrees of freedom that capture the essential physics of the process under study. In this talk, I will discuss how these problems can be addressed using machine learning approaches. The freezing transition will serve as illustrative example.