



# CALL FOR PAPERS

**ICSMD 2021**  
**Mar 04-05, 2021**  
**Rio de Janeiro, Brazil**

The International Research Conference is a federated organization dedicated to bringing together a significant number of diverse scholarly events for presentation within the conference program. Events will run over a span of time during the conference depending on the number and length of the presentations.

ICSMD 2021 : International Conference on Scalable Molecular Dynamics is the premier interdisciplinary forum for the presentation of new advances and research results in the fields of Scalable Molecular Dynamics. The conference will bring together leading academic scientists, researchers and scholars in the domain of interest from around the world. Topics of interest for submission include, but are not limited to:

Molecular engineering	Semi-empirical potentials
Molecular geometry	Polarizable potentials
Molecular dynamics	Potentials in ab initio methods
Protein function	Hybrid QM/MM
Physical movements of atoms and molecules	Coarse-graining and reduced representations
Design constraints	Steered molecular dynamics (SMD)
Microcanonical ensemble (NVE)	Examples of applications
Canonical ensemble (NVT)	Molecular dynamics algorithms
Isothermal-isobaric (NPT) ensemble	Integrators
Generalized ensembles	Short-range interaction algorithms
Potentials in MD simulations	Long-range interaction algorithms
Empirical potentials	Parallelization strategies
Pair potentials versus many-body potentials	Specialized hardware for MD simulations