

*Axiomata
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Leges Motus*



Seminar über Fragen der Mechanik

zu folgendem Vortrag wird herzlich eingeladen

Donnerstag, **28.05.2009, 16:00 Uhr**, Egerlandstr. 5, Raum 0.044

Charting energy landscapes by molecular dynamics

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Outline

0. Looking at energy landscapes: intermolecular potentials and energy functionals
1. The (Andersen-)Parrinello-Rahman Molecular Dynamics
2. How to justify the P-R kinetic energy
3. What metadynamics makes sense to explore energy landscapes
4. Micro/Macro consistency: zero-temperature P-R MD and the Cauchy-Born Rule