Statistical Physics Seminar

May 9th, 2018.
Wednesday, 11.00

ELTE TTK Northern Building 2.54

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From the potential to the phase diagram using nested sampling

We use the nested sampling algorithm, a recently developed density-of-states technique, to calculate the partition function of real materials. It can be used to efficiently determine the complete equilibrium phase diagram corresponding to a given atomistic potential energy function in a highly automated fashion. The only inputs required are the composition and the desired pressure and temperature ranges, and, in particular, solid-solid phase transitions are recovered without any a priori knowledge about the structure of solid phases.

Phys. Rev. E 96, 043311 (2017) Constant-pressure nested sampling with atomistic dynamics
Phys. Rev. B 93, 174108 (2016) Determining pressure-temperature phase diagrams of materials
Phys. Rev. E 89, 022302 (2014) Nested sampling for materials: The case of hard spheres
J. Phys. Chem. B 114, 10502 (2010) Efficient Sampling of Atomic Configurational Spaces

1117. Budapest, Pázmány Péter sétány 1/A (Északi tömb)
Room 2.54
http://glu.elte.hu/~statfiz/index.html