The Frenkel-Kontorova Chain

W. Quapp and J. M. Bofill

Mathematisches Institut, Universität Leipzig, PF 100920, D-04009 Leipzig, and Departament de Química Inorgànica i Orgànica, Secció de Química Orgànica, and Institut de Química Teòrica i Computacional, (IQTCUB), Universitat de Barcelona, Martí i Franquès 1, 08028 Barcelona, Spain

Abstract

Newton trajectories[1] are used for the Frenkel-Kontorova model of a finite molecular chain with free-end boundary conditions enbedded in a side potential. Thus the model has two competing potentials and it has an interesting potential energy surface. We optimize stationary structures, and we search the lowest energy saddle points for a complete minimum energy path for a movement of the chain over the full period of the on-site potential, a sliding of the chain over the substrate.[2,3]

A central role plays a saddle point of index 2, a low summit[4] in the mountains.

Newton trajectories are an ideal tool to understand the circumstances under a driving of a Frenkel-Kontorova chain by external forces. For special directions of the external force, the corresponding Newton trajectory follows the minimum energy path through the PES. Such external forces can cause a sliding of the full chain which may be named done by superlubricity.

If the tilting is set, then one is interested in barrier breakdown points on the potential energy surface for a critical tilting force named the static frictional force.

We explain the theory and demonstrate it with an example.

[1] W. Quapp, J.M. Bofill, J. Ribas-Ariño: Int.J.Quant.Chem. **118**, 2018, e25775 "Towards a Theory of Mechanochemistry – Simple Models from the Early Beginnings"

[2] W. Quapp, J.M. Bofill, Mol.Phys. doi.org/10.1080/00268976.2019.1576930 2019, "Newton Trajectories for the Frenkel-Kontorova Model"

[3] W. Quapp, J.M. Bofill, Europ.Phys.J. submitted "A Model for a Driven Frenkel-Kontorova Chain"

[4] D. Heidrich, W. Quapp, Theor.Chim.Acta **70**, 89 (1986) "Saddle points of index 2 on PES and their role in theoretical reactivity investigations"