On behalf of the

Science College CMS
Vienna Computational Materials Laboratory
and Center for Computational Materials Science

we cordially invite you to the following seminar

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High-Dimensional Neural Network Potential-Energy Surfaces for Atomistic Simulations

The reliability of the results obtained in molecular dynamics simulations strongly depends on the quality of the employed interatomic potentials. While electronic structure methods like density-functional theory (DFT) provide an accurate description of many systems, the high computational costs limit the system size that can be studied. Therefore, the development of more efficient, approximate potentials is a very active field of research.
In recent years artificial Neural Networks (NN) have become a valuable new tool to represent ab initio potential-energy surfaces (PES) very accurately [1,2]. In general, NNs are a class of very flexible and unbiased functions, which do not require any knowledge about the physical nature of the atomic interactions. They can be applied to interpolate a set of DFT reference points and then allow to calculate the energy and forces several orders of magnitude faster with almost the accuracy of the underlying electronic structure data. Most applications published in the literature to date present NN potentials for PESs of small molecules. However, a few years ago, the NN method has been extended to high-dimensional potential-energy surfaces thus now enabling molecular dynamics studies of very large condensed systems [3,4]. Several NN potentials for molecules, clusters and bulk materials are presented to demonstrate that a very high accuracy can be obtained for a wide range of systems. The efficiency of the NN potentials provides access to physical problems, which cannot be studied directly by DFT.

[1] T.B. Blank, S.D. Brown, A.W. Calhoun, and D.J. Doren, J. Chem. Phys. 103, 4129 (1995).
[2] S. Lorenz, A. Groß, and M. Scheffler, Chem. Phys. Lett. 395, 210 (2004).
[3] J. Behler, and M. Parrinello, Phys. Rev. Lett. 98, 146401 (2007).
[4] N. Artrith, T. Morawietz, and J. Behler, submitted (2011).

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