About CPMD2017

CPMD2017 Local Organizing Committee[1,*]
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Car-Parrinello Molecular Dynamics (CPMD) [1] and *ab initio* molecular dynamics have become a widespread tool in atomistic simulations of materials and molecular systems in a variety of fields, covering physics, chemistry, biochemistry and materials science. The CPMD2017 [2] will bring together developers and practitioners in the field of ab initio MD, to discuss state-of-the-art methodological developments as well as applications. Besides, CPMD2017 will also focus on data-driven / machine-learning approaches, emerging in the materials science field rapidly. Interactions among the researchers in these fields will give a future direction of computational materials / molecular science. The meeting consists of oral talks by keynote and invited speakers as well as poster presentations by general participants. The CPMD2017 is the first CPMD workshop in the Asian region.

Fig. 1: CPMD2017 logo, which symbolically represents the fictitious mass μ, a free energy profile (upside-down), and Mt. Tsukuba.

[1] R. Car and M. Parrinello, *Phys. Rev. Lett*. **55**, 2471 (1985).
[2] CPMD2017 web site, http://www.nims.go.jp/MII-I/CPMD2017/