高分子科学系列讲座

高分子物理与化学国家重点实验室 中国科学院长春应用化学研究所

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报告题目	**Fast Monte Carlo Simulations: Combining and Comparing Particles with Fields**		

内容摘要

The basic idea of fast Monte Carlo (FMC) simulations [*Q. Wang and Y. Yin*, **J. Chem. Phys. 130**, 104903 (2009); *Q. Wang*, **Soft Matter 5**, 4564 (2009); *ibid.* **6**, 6206 (2010)] is to use soft potentials that allow particle overlapping, instead of hard-core repulsions (e.g., the Lennard-Jones potential or the self- and mutual-avoiding walk) as in conventional molecular simulations. This gives orders of magnitude faster/better sampling of configuration space. More significantly, using soft potentials is the only way to study experimentally accessible fluctuations in dense polymeric systems. Furthermore, since soft potentials are commonly used in polymer field theories, using the same Hamiltonian in both FMC simulations and the theories enables stringent test of the latter, without any parameter-fitting, to unambiguously quantify the consequences of theoretical approximations. In this talk I will use several systems to demonstrate these great advantages of FMC simulations, performed either in continuum or on a lattice.