Coarse grain modeling of liquid methyl methacrylate

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Résumé en anglais	We implement a coarse graining procedure in order to construct a simple intermolecular potential model for liquid (poly)methyl methacrylate (P)MMA. The procedure and the potential model obtained thereby aim at building an effective input towards accelerated molecular-dynamics calculations as well as a simpler statistics for oncoming simulations of MMA and PMMA melts. As a result, atomistic description of the molecule is substantially simplified while preserving as many properties of the original substance as possible. The hard core of the approach consists in optimizing iteratively a typical Lennard-Jones (6-12) potential until the radial distribution function generated from the coarse grained model becomes consistent with the atomistic target function. The new model allows one to make an economy by one order of magnitude in the CPU time.
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