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Monte Carlo simulation of highly oxidized oligopyrroles in condensed phases[1] WEIXIAO JI, CLIFFORD HALL, ESTELA BLAISTEN-BAROJAS, Computational Materials Science Center, George Mason University, Fairfax, VA — We present a new classical model potential for the simulation of oxidized oligopyrroles. The novel potential treats the monomers as rigid bodies interacting through covalent, bending, torsion, dipole-dipole, anti-coiling, excluded volume and coulomb interactions. The potential contains 24 parameters fitted on a database of energy points calculated at the density functional theory quantum approach. Studies include structural and mechanical properties of condensed phase systems composed of 1188 pyrrole oligomers with 12 monomers each and 4752 electronegative atoms yielding a 33% dopant concentration. The mechanical equilibrium density is determined by isothermal-isobaric Monte-Carlo. The equilibrium configurations at various temperatures are studied in the canonical ensemble and our Adaptive Tempering Monte Carlo (ATMC), a multi-canonical ensemble method, finds the global minimum of the energy. Binding energy, end-to-end distance, radius of gyration, vector and orientation order parameters, and pair correlation functions are reported at 300K and 1000K.A new computational algorithm in CUDA allows a significant computer acceleration using GPUs. With this novel implementation we obtain speedup of a 45-factor faster than CPU at sufficiently large system sizes.

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