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A novel soft-core spherocylinder model for liquid crystals JING ZONG, XINGHUA ZHANG, QIANG WANG, Department of Chemical and Biological Engineering, Colorado State University — Interaction models with soft-core repulsions that allow particle overlapping give orders of magnitude faster/better sampling of configurational space than those with hard-core repulsions (e.g., hard spherocylinders or Gay-Berne potential). While several soft-core spherocylinder models were recently proposed[1], their repulsive interaction depends only on the shortest distance between two spherocylinders. Here we present a novel, computationally efficient soft-core spherocylinder model, which gives exact treatment of the excluded-volume interactions and anisotropic shape of two particles (thus the orientational interaction between them favoring their parallel alignment). It further takes into account the degree of overlap between the two particles, thus superior to other soft-core models. This model has great potential applications in the study of liquid crystals, block copolymers containing rod blocks, and liquid crystalline polymers. [1] *Z. E. Hughes et al.*, **Comput. Phys. Commun., 178**, 724 (2008); *J. S. Lintuvuori and M. R. Wilson*, **J. Chem. Phys., 128**, 044906 (2008).

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