



Modification of the Gay-Berne potential for improved accuracy and speed

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A modification of the Gay-Berne potential is proposed which is about 10% to 20% more speed efficient (that is, the original potential runs 15% to 25% slower, depending on architecture) and statistically more accurate in reproducing the energy of interaction of two linear Lennard-Jones tetratomics when averaged over all orientations. For the special cases of end-to-end and side-by-side configurations, the new potential is equivalent to the Gay-Berne one.

Comments: 5 pages (incl. title page), [preprint,aip,jcp]{RevTEX-4.1}, 1 figure, 1 table. Revised version fixes mathematical typos and adds short paragraph on a natural generalization to dissimilar particles

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