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Generalized Stacking Fault Energies in the Basal Plane of Triclinic Molecular Crystal 1,3,5-Triamino-2,4,6-Trinitrobenzene (TATB) NITHIN MATHEW, THOMAS SEWELL, University of Missouri-Columbia — Molecular dynamics and molecular mechanics simulations were used in conjunction with a fully flexible force field to calculate the generalized stacking fault energies in the basal plane (that is, the $a - b$ plane, where a, b, and c define the edge vectors of the primitive unit cell) of the triclinic molecular crystal 1,3,5-triamino-2,4,6-trinitrobenzene (TATB). Crystal symmetry and molecular stacking arrangement result in two glide plane types for the same glide plane normal vector. The unstable stacking fault energies are found to be less than 10 $\mathrm{mJ/m^2}$ at 0 K and atmospheric pressure, indicating easy dislocation glide. Glide in the a and $a - b$ directions are favored to that in the b direction. Asymmetric unstable stacking fault energies indicate an asymmetric barrier to dislocation glide. Stable stacking faults with energies less than 1 $\mathrm{mJ/m^2}$ are predicted for the a and $a - b$ directions. A compound twin is observed in the a direction with energy of 2.52 $\mathrm{mJ/m^2}$. Nitro (NO_2) groups on the molecules undergo out-of-plane rotations during glide. The extremely small barriers to twinning and dislocation glide might be sources for observed second harmonic generation in the nominally centrosymmetric crystal.

Thomas Sewell
University of Missouri-Columbia

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