

Abstract Submitted
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Exfoliation of stacked sheets: effects of temperature and platelet size by a Monte Carlo simulation¹ BARRY FARMER, Air Force Research Laboratory, RAS PANDEY, University of Southern Mississippi — Can a layer of stacked sheets (coarse grained description of clay platelets) exfoliate in a solvent? Computer simulations are performed to address this question with a stacked layer of four sheets. A sheet is modeled by nodes tethered together by fluctuating bonds on a cubic lattice; sheets of sizes $12^2 - 64^2$ are considered. The initial distance between sheets is small and kept constant for different sets of stacked sheets. There is an attractive interaction between sheets, i.e., their nodes and the empty lattice sites, the effective solvent medium. Nodes execute stochastic movement with the Metropolis algorithm subject to bond fluctuation and excluded volume constraints. Simulations are performed at different temperatures. Visual analysis shows that the exfoliation depends on the size of the sheet and temperature. We find that it is easier to exfoliate smaller sheets and that the exfoliation is enhanced by raising the temperature. The exfoliation becomes very slow for large sheets at low temperatures due to longer relaxation times.

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