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Exfoliation and intercalation in a layer of clay platelets: effects of solvent and temperature by a Monte Carlo simulation BARRY FARMER, Air Force Research Laboratory, RAS PANDEY, University of Southern Mississippi — Effects of the quality of solvent and temperature on the exfoliation of a layered platelets and intercalation of solvent are studied by a Monte Carlo simulation. A platelet is modeled by square sheet consisting of nodes tethered together by fluctuating bonds on a cubic lattice. A stack of four sheets constitutes the layer with a small initial inter-layer distance. A fraction of the lattice sites are randomly occupied by the solvent particles initially; a solvent constituent is modeled by a particle with the size of a node. The interaction strength (attractive and repulsive) between sheet nodes and the solvent particles control the quality of the solvent. Solvent constituents and sheet nodes execute stochastic movement with the Metropolis algorithm subject to bond fluctuation and excluded volume constraints. Density profiles of the sheet and solvent particles and their dynamics are studied for a range of temperatures in different solvent media. The quality of solvent plays a critical role in exfoliation of sheets and intercalation of solvent constituents between the sheet layers particularly at low temperatures. The exfoliation is enhanced on increasing the temperature.

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