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Cleavage Energies of Modified Layered Silicates by Molecular Dynamics Simulation YAO-TSUNG FU, HENDRIK HEINZ, Department of Polymer Engineering, University of Akron — The cleavage energy of organically modified layered silicates indicates the thermodynamic propensity of exfoliation in polymer matrices. We find substantial cleavage energy differences upon variation in cation exchange capacity (CEC) (90 and 145 meq/100g), head groups (-NH_3 and –NMe_3), and chain length of the surfactants (C2 to C14) due to layering effects of the surfactants in the galleries using molecular dynamics simulation. Model systems of full atomistic detail are periodic in the xy plane, open in the z direction, are subjected to sheet separation starting at equilibrium distance. Overall, the cleavage energy, consistent with experimentally measured surface tensions and previous calculations for selected organoclays, shows complex fluctuations as a function of chain length and head group structure. Computed cleavage energies are in the range 25-50 mJ/m^2 for C2$\sim$C14 (-NH_3 headgroup) and 40-200 mJ/m^2 for C2$\sim$C14 (–NMe_3 headgroup) at two CEC layered silicates. The progression is not linear and related to the packing density of the interlayer of self-assembled surfactant chains and surface reconstruction of the modified layered silicates upon cleavage.

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