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Molecular Simulation of MoS_2 Exfoliation[1] GUOQING ZHOU, RAJIV KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, Univ of Southern California — Liquid exfoliation is widely used to synthesize a variety of two-dimensional materials such as graphene and atomically thin layers of boron nitride and transition metal dichalcogenides. We perform molecular dynamics (MD) simulations to study the mechanism of exfoliation in MoS_2. The wettability of water and water/2-propanol (IPA) on MoS_2 is investigated and the results are compared with experimental data on interfacial energies to fit the force fields of the MD simulation. With the optimized force fields, we perform shock simulations of nanobubble collapse and study the generation of high speed nanojets from nanobubble collapse in the water/IPA mixture. Results will be reported on the exfoliation of MoS_2 into atomically thin layers by the impact of nanojets.

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