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If it won't explode, hit it with a hammer: Facilitating chemical reactions at a liquid surface

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Collisional energy transfer at a gas-liquid interface may play an important role in the initial decomposition of multiphase combustibles. The energy feedback of hot, energetic, gaseous atoms, in this case Ar, striking the liquid surface can potentially impart enough energy to break one of the liquid's bonds in a homolytic fashion thus creating radicals necessary for a resulting explosive chain reaction. Liquid nitromethane (CH_3NO_2) is a prototypical explosive and is modeled here as a simple diatomic consisting of one methyl (CH_3) and one nitro (NO_2) groups. The methyl and nitro groups are shown through MP2 6-311+G (2d, 2p) calculations to be the most likely resulting decomposition fragments; as such, focus is placed on the breaking of the C-N bond. For this study, the attractive term of the gas-liquid interaction potential is assumed to be zero to find the limit of Ar-nitromethane interaction. The energy transfer is studied by running simulations, using the DL_Poly_2 program, of Ar impinging the liquid nitromethane from zero degrees to the surface normal and over multiple incident energies. The results are then analyzed for energy transfer and C-N bond breakage.