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Creating reactive potentials for particle-surface interactions: C, H, Li[1] P.S. KRSTIC, P. KENT, ORNL — The reliability of the molecular dynamic simulations of particle-surface interactions strongly depends on the quality of the ground electronic state potentials which determine classical forces for dynamics of all heavy particles particles in the system. Using multidimensional optimization techniques we improve the quality of the existing hydrocarbon potentials [Brenner et al, J. Phys: Condens. Matter 14, 783 (2002)] for the close-nuclei encounters. In addition, we present initial results for a new potential developed for carbonized lithium surfaces and apply for both chemical and physical sputtering yields.

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