Abstract Submitted
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Molecular Dynamics of Lithium-Carbon Surfaces[1] P.S. KRSTIC, Oak Ridge National Laboratory, E. YANG, Purdue University, J. DADRAS, University of Tennessee, P. KENT, Oak Ridge National Laboratory, A. ALLOUCHE, CNRS, J.P. ALLAIN, Purdue University — We study chemistry induced by low-energy deuterium impact of lithiated carbon surface. The processes include evolution of the lithium-carbon surfaces as well as chemical sputtering. New interatomic potentials are developed for the molecular dynamics simulations of the mixed Li-C-H material, based on the Brenner-Tersoff form, with Lenard-Jones corrections. Particular attention is paid to the Coulomb interactions of the charged atoms in this mixed material induced by large difference in the electronegativity of lithium and carbon-hydrogen. We compare our results with available experimental data.

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