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ELECTRONIC, STRUCTURAL AND THERMODYNAMIC PROPERTIES OF ICOSAHEDRAL FREE AND DEPOSITED Al CLUSTERS ON AL SURFACES FROM TIGHT BINDING AND MOLECULAR DYNAMICS SIMULATIONS

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Icosahedral Al clusters made of 55, 147 and 309 particles were studied by means of Tight Binding zero temperature calculations and Molecular Dynamics simulations. We focus on the properties of the free and also of the deposited clusters on the low indexed Al surfaces. From these computations we deduced several quantities related to the electronic, structural and thermodynamic properties of the free clusters, like electronic densities of states, phonon densities of states and melting points, while we found that the deposited clusters reconstruct very quickly adopting the substrate's structure and orientation