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Theoretical Study of Na3-C60 and Na4-C60 Clusters: Pathways to Nanoscale Contacts DANIEL BULNES, NICHOLE MOYA-LEYBA, ERICA VELARDE, AJIT HIRA, Northern NM Community College — We continue our interest in fullerene-alkali complexes[1−2] by investigating the physical and chemical properties of Na_3-$C_{60}$and Na_4-C_{60} systems. Five categories of adsorption sites for the alkali atoms on the fullerene molecule, namely fivefold, threefold, midbond-long, midbond-short and top, are considered. Electron correlation effects, using both Many Body Perturbation Theory (MBPT) and Density Functional Theories (DFT) are incorporated in the calculations for binding energies and optimal intermolecular bondlengths. For these complexes, various properties including bondlengths, ground-state energies, optimum absorbate distances, dissociation channels, and dissociation energies are presented. Possibility of tunneling between different sites is investigated. We also examine implications for the fabrication of nanoscale contacts, and for the study of dynamical systems involving C_{60}.

1. A. S. Hira and A. K. Ray, Phys. Rev. **A 52**, 141(1995); **A 54**, 2205(1996).

2. A. S. Hira, Billy Terrazas, Erica Velarde and Desirae Vigil, "An *Ab Initio* Theoretical Study of Alkali-C_{60} and Alkali-$(C_{60})_n$ Clusters," Bull. Am. Phys. Soc. **49**, 599 (March 2004).

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