Site-specific polarizabilities as predictors of optimal binding sites of H$_2$O on Na$_n$ clusters[1] LI MA, KOBLAR JACKSON, Physics Dept., Central Michigan University, Mount Pleasant, MI 48859, JULIUS JELLINEK, Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne IL 60439 — We have used density functional theory (DFT), in the generalized gradient approximation to study the adsorption of water molecules on sodium clusters, Na$_n$, for n = 7, 12, 18, and 25. These clusters span a range of sizes and surface topographies. In each case, we conduct an extensive search to identify the optimal binding site of the ad-molecule on the cluster. We analyze the results within the framework of cluster polarizabilities, making use of a new methodology for partitioning the cluster polarizability into atomic components (Jackson et al., J. Chem. Phys. **129**, 144309 (2008)). We show that the most favorable adsorption sites are at surface atoms that have the largest atomic polarizabilities. We will compare and contrast these results with corresponding findings for the adsorption of O$_2$ and NH$_3$ molecules on Na$_n$ clusters.

Koblar Jackson
Physics Dept., Central Michigan University, Mount Pleasant, MI 48859

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