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Origin of electric dipole moments in free niobium clusters KRISTOPHER ANDERSEN, UC Davis, VIJAY KUMAR, YOSHIYUKI KAWAZOE, Tohoku University, Japan, WARREN PICKETT, UC Davis — Niobium clusters Nb_n ($5 \leq n \leq 200$) with surprisingly large, spontaneous electric dipole moments were recently observed in low-temperature ($T < 100$ K) molecular beam experiments by Moro *et al.* (Science **300**, 1265). We address the origin of the electric dipole using first-principles electronic structure calculations for Nb_n ($n \leq 15$). The calculated moments generally agree with the experimental data, in which negligible moments are found for $n = 4$, 10, and 15; moderate moments for $n = 5$–9; and large moments for $n = 11$–14. A strong correlation is found between the geometrical asymmetry of the cluster and electric dipole: its magnitude is proportional to the spread in the principal moments of inertia and its direction tends to align along the axis of the largest principal moment. Charge deformation densities reveal directional, partially covalent bonds that stabilize the structural asymmetry. Classical simulations of the deflection of a cluster in a molecular beam provide evidence that the electronic dipole may persist at higher temperatures, but is masked by the rotational dynamics of the cluster.

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