Abstract Submitted
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Two-level tunneling systems in amorphous alumina[1] IRINA V. LEBEDEVA, ALEJANDRO P. PAZ, ILYA V. TOKATLY, ANGEL RUBIO, Nanobio Spectroscopy Group and ETSF Scientific Development Centre, Universidad del Pais Vasco, Spain — The decades of research on thermal properties of amorphous solids at temperatures below 1 K suggest that their anomalous behaviour can be related to quantum mechanical tunneling of atoms between two nearly equivalent states that can be described as a two-level system (TLS) [1]. This theory is also supported by recent studies on microwave spectroscopy of superconducting qubits [1]. However, the microscopic nature of the TLS remains unknown. To identify structural motifs for TLSs in amorphous alumina we have performed extensive classical molecular dynamics simulations. Several bistable motifs with only one or two atoms jumping by considerable distance $\sim$ 0.5 Å were found at T=25 K. Accounting for the surrounding environment relaxation was shown to be important up to distances $\sim$ 7 Å. The energy asymmetry and barrier for the detected motifs lied in the ranges 0.5 - 2 meV and 4 - 15 meV, respectively, while their density was about 1 motif per 10 000 atoms. Tuning of motif asymmetry by strain was demonstrated with the coupling coefficient below 1 eV. The tunnel splitting for the symmetrized motifs was estimated on the order of 0.1 meV. The discovered motifs are in good agreement with the available experimental data.

[1] G. J. Grabovskij et al. Science 338, 232 (2012)

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