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First-Principles Analyses of Capacitance and Conductance of Atomic Point Contacts MICHIKO TANAKA, SHINNOSUKE FURUYA, SATOSHI WATANABE, Department of Materials Engineering, The University of Tokyo and CREST-JST — Conductance of atomic point contacts has been actively examined. On the other hand, there are only few investigations on their capacitance in the atomic scale, and thus its behavior has not been understood sufficiently yet. Here, we examine the capacitance of atomic point contacts together with their conductance. To calculate electronic states under applied bias voltages self-consistently, we adopt the boundary-matching scattering-state density functional method developed by our group. We investigate three models: (a) Two Al (100) electrodes with attached Al pyramidal clusters, (b) Al electrode with an attached Al pyramidal cluster and flat Al electrode, and (c) two flat Al electrodes. We found that the behavior of capacitance depends on structure: In (a) and (c), the capacitance first increases and then decreases with the increase in inter-electrode distance, while it shows a monotonic decrease in (b). For the conductance, our calculation reproduces the observed behavior that during stretching processes the conductance increases just before breaking of the contact in (a).

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