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Quantum Size Effect and Electronic Stability of Freestanding Metal Atom Wires[1] HAIPING LAN, PING CUI, U. of Sci. & Tech. of China, JUN-HYUNG CHO, Hanyang U., QIAN NIU, U. of Texas at Austin, JINLONG YANG, U. of Sci. & Tech. of China, ZHENYU ZHANG, Oak Ridge Nat. Lab, U. of Tennessee, U. of Sci. & Tech. of China — Using DFT calculations, we present a thorough study of the quantum size effects on the stability of freestanding metal atom wires. Our systems include Na, Ag, Au, In, Ga and Pb atom wires, i.e. s, sd, and sp electron prototypes. We found that the total energy always oscillates with the wire length, which clearly indicates the existence of preferred lengths. Increasing the length, the s-system exhibits even-odd oscillations following a 1/x decay law in the stability, which can be attributed to electron band filling and quantum confinement along the wire. The sd-system exhibits a similar oscillation pattern, even in the presence of sd hybridization. In sp-system, the energy oscillations are beyond the simple even-odd nature, likely due to unpaired p orbitals and the corresponding nontrival band filling. Our findings clearly demonstrate that electronic contribution is quite critical to the stability of freestanding wires, and this stability may be important even when wires are deposited on substrates or strained. This study sheds light on the underlying formation mechanism of metal atom wires.

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