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Does aluminum conduct better than copper at the nanoscale? A first-principles study of metallic nanowires[1] ADAM SIMBECK, NICK LANZILLO, NEERAV KHARCHE, SAROJ NAYAK, Rensselaer Polytechnic Institute — From first-principles, we present a theoretical and comparative investigation of the role of quantum confinement in altering the electronic, transport, and phonon properties of linear, single-atom thick chains, i.e. nanowires, of metallic (Au, Ag, Cu, and Al) atoms. Our results for the ballistic quantum transport properties and electronic structure are in perfect agreement with those previously published. Motivated by this, we also consider electron-phonon interactions in such devices, where we report an order of magnitude reduction in the electron-phonon coupling constant for Al, whereas an enhancement is predicted for Au, Ag, and Cu.

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