

Abstract Submitted  
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**Electronic Structure of Metal-Semiconductor Nanocontacts**<sup>1</sup> DENIS DEMCHENKO, LIN-WANG WANG, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 — Future nanoelectronics will depend on the electron/hole transport in a nanostructure and across nanostructure/metal electrode interfaces. Measurements of nanoscale transport are often conducted by contacting a semiconductor nanostructure with large metallic electrodes. Theoretical interpretation of such experiments, however, is often based on electronic structure of an isolated nanostructure, ignoring the influence of the electrodes. Here we address this issue by calculating the classical electrostatic polarization potential  $P(r)$ , and incorporating it into the atomistic pseudopotential method, to calculate the electronic structure of experimentally-relevant sizes of nanorods. We calculate several electrode/nanorod geometries, with varying contact depths. We show that the presence of an electrode can produce localized electron and hole states near the electrode. The localization is caused by the spatial variation of the  $P(r)$ . We have calculated the effects of the applied bias necessary to overcome the electron/hole localization, as well as the change of the band gap and the binding energy of the localized state as functions of the nanorod-electrode separation.

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