

Pseudopotential calculations 25 years after Kleinman-Bylander

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“Pseudopotential-density functional theory” provides one of the most popular approaches to calculate the electronic and structural properties of materials. A key advance in this approach was the creation of an “efficient form for model pseudopotentials,” as described in a paper published by Kleinman and Bylander in *Physical Review Letters* **48**, 1425 (1982). This seminal paper has played a dramatic role in the construction of contemporary pseudopotentials and continues to be widely cited with over 3,000 citations to date. In this presentation, I will illustrate some recent work based on the Klein-Bylander pseudopotential form in real space calculations for the electronic properties of solids, nanostructures, clusters and liquids.