The Evolution of the Pseudopotential Method for Computational Materials Science

Marvin L. Cohen

Department of Physics
366 Le Conte Hall MC #7300
University of California, Berkeley
Berkeley, CA 94720

and

Materials Sciences Divison
Mailstop: 19-366
Lawrence Berkeley National Laboratory
Berkeley, CA 94720

phone (510) 642-4753; fax (510) 643-9473; mlcohen@berkeley.edu

Abstract: A general discussion will be given of the background related to the development of pseudopotential theory from Fermi's original work to its use in current computational approaches to study materials. The evolution from calculations for electronic and structural properties of bulk materials, surfaces, and interfaces, to predicting properties like superconductivity will be described. The motivating concepts will be emphasized, and a description of some current activities will be given with a focus on the properties of nanostructures. The influence of Roberto Car's contributions, particularly the Car-Parrinello Method, will be discussed.