



## Pseudopotential and all electron atomic core size scales

Alex Zunger

Citation: [The Journal of Chemical Physics](#) 74, 4209 (1981); doi: 10.1063/1.441556

View online: <http://dx.doi.org/10.1063/1.441556>

View Table of Contents: <http://scitation.aip.org/content/aip/journal/jcp/74/7?ver=pdfcov>

Published by the [AIP Publishing](#)

---

Articles you may be interested in

[Norm-conserving pseudopotentials with chemical accuracy compared to all-electron calculations](#)

*J. Chem. Phys.* 138, 104109 (2013); 10.1063/1.4793260

[Theoretical investigation of the alkaline-earth dihydrides from relativistic all-electron, pseudopotential, and density-functional study](#)

*J. Chem. Phys.* 126, 104307 (2007); 10.1063/1.2437213

[All-electron and relativistic pseudopotential studies for the group 1 element polarizabilities from K to element 119](#)

*J. Chem. Phys.* 122, 104103 (2005); 10.1063/1.1856451

[The accuracy of the pseudopotential approximation. III. A comparison between pseudopotential and all-electron methods for Au and AuH](#)

*J. Chem. Phys.* 113, 7110 (2000); 10.1063/1.1313556

---





<sup>4</sup>H. Weinstein, P. Politzer, and S. Serbernik, *Theor. Chem. Acta* **38**, 159 (1975).

<sup>12</sup>M. Schlüter, A. Zunger, G. P. Kerker, K. M. Ho, and M. L. Cohen, *Phys. Rev. Lett.* **42**, 540 (1979); G. P. Kerker, A. Zunger, M. J. Cohen, and M. Schlüter, *Solid State Com.*