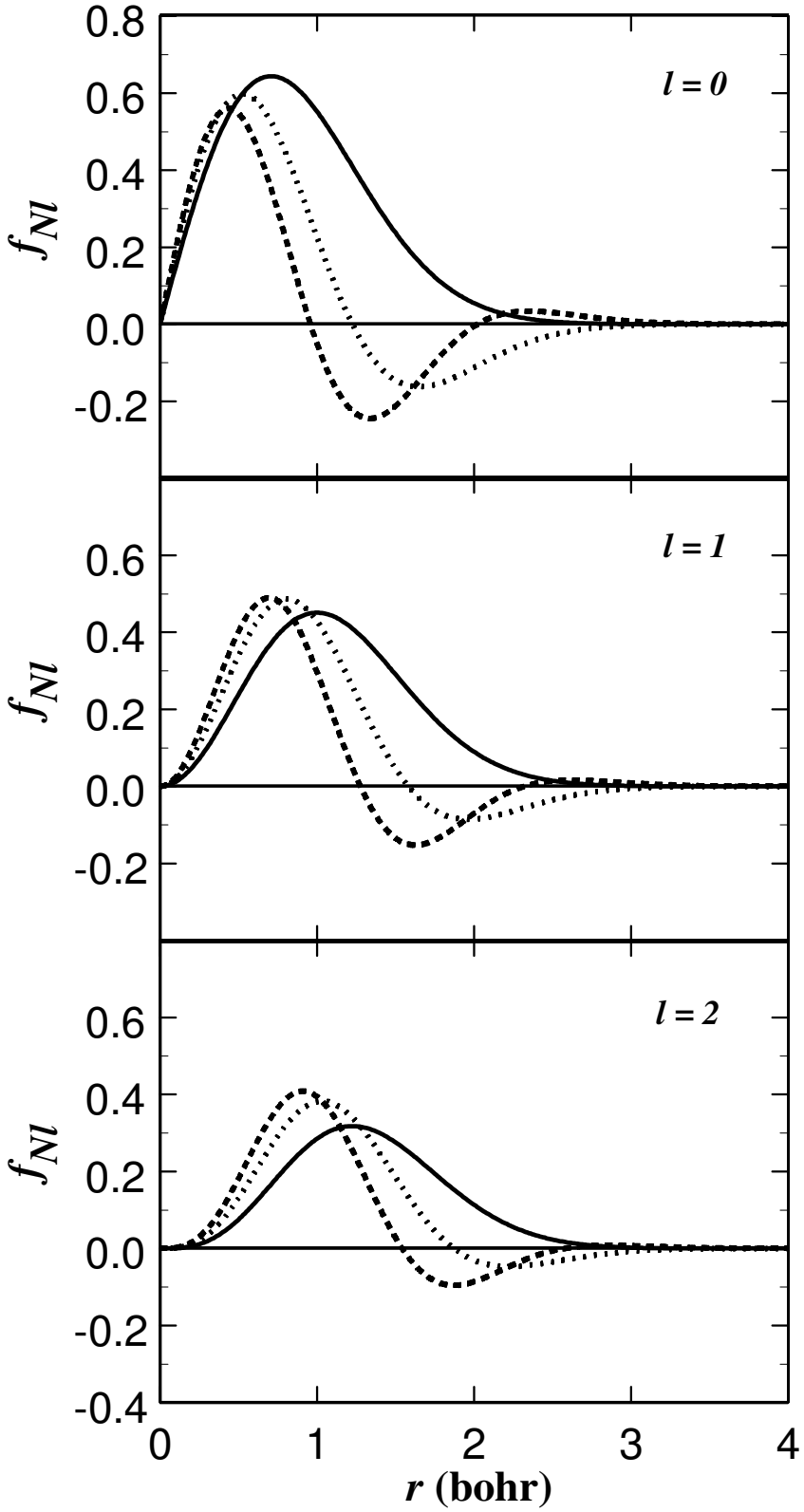


Figure 1: Plots of the projector basis functions defined in Eq. (8) for $\sigma = 1$ and $N = 0$ (solid line), 1 (dashed line), and 2 (dotted line).

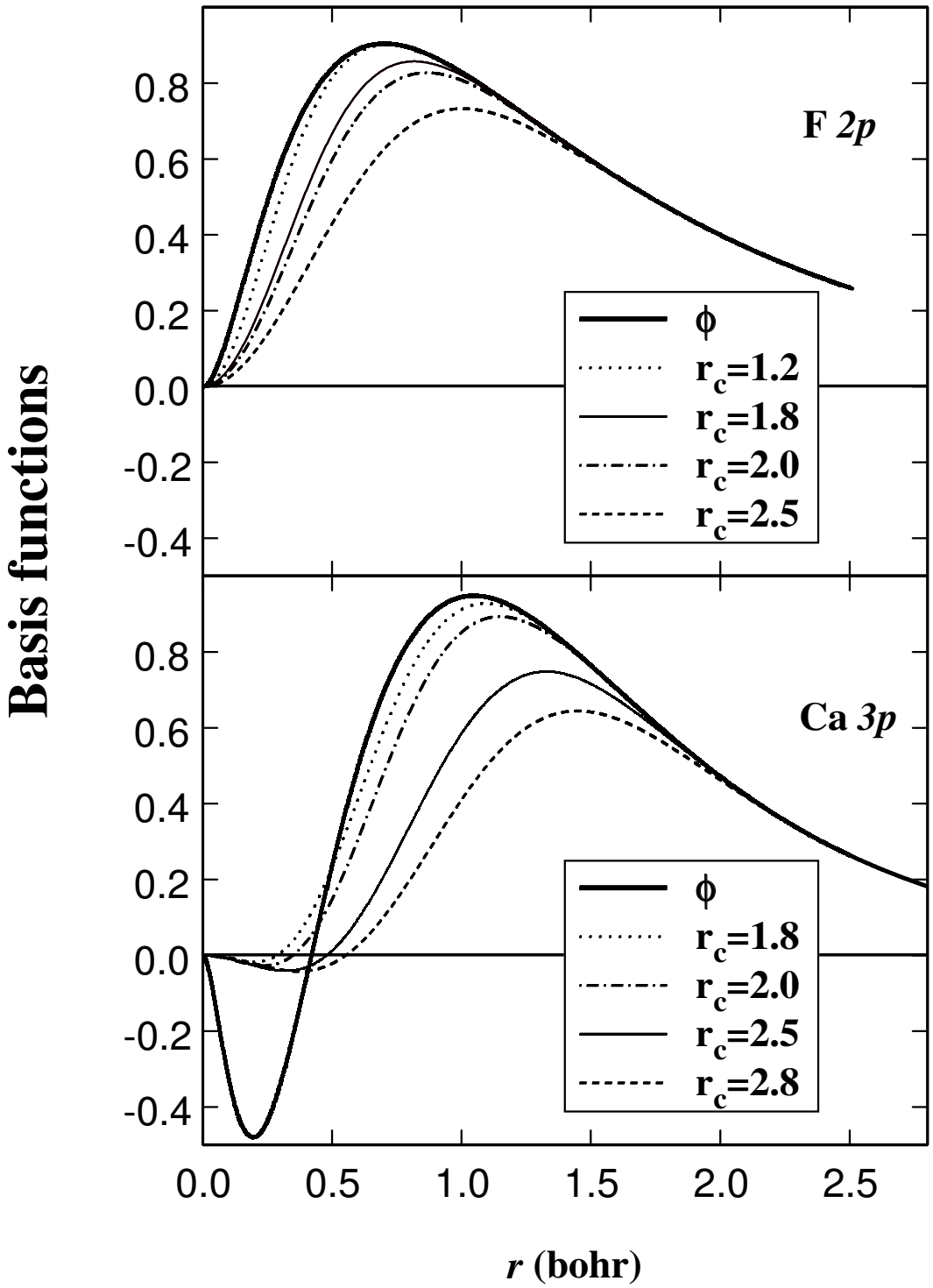


Figure 2: Comparison of PS basis functions constructed with various values of $r_c$ with $V_0 \equiv 0$. Top panel shows F functions $\tilde{\phi}^F_{2p}$ for $r_c = 1.2$, 1.8, 2.0, and 2.5 bohr with the AE function $\phi^F_{2p}$ included with a thick line for comparison. Bottom panel shows Ca functions $\tilde{\phi}^{Ca}_{3p}$ for $r_c = 1.8$, 2.0, 2.5, and 2.8 bohr with the AE function $\phi^{Ca}_{3p}$ included with a thick line for comparison.

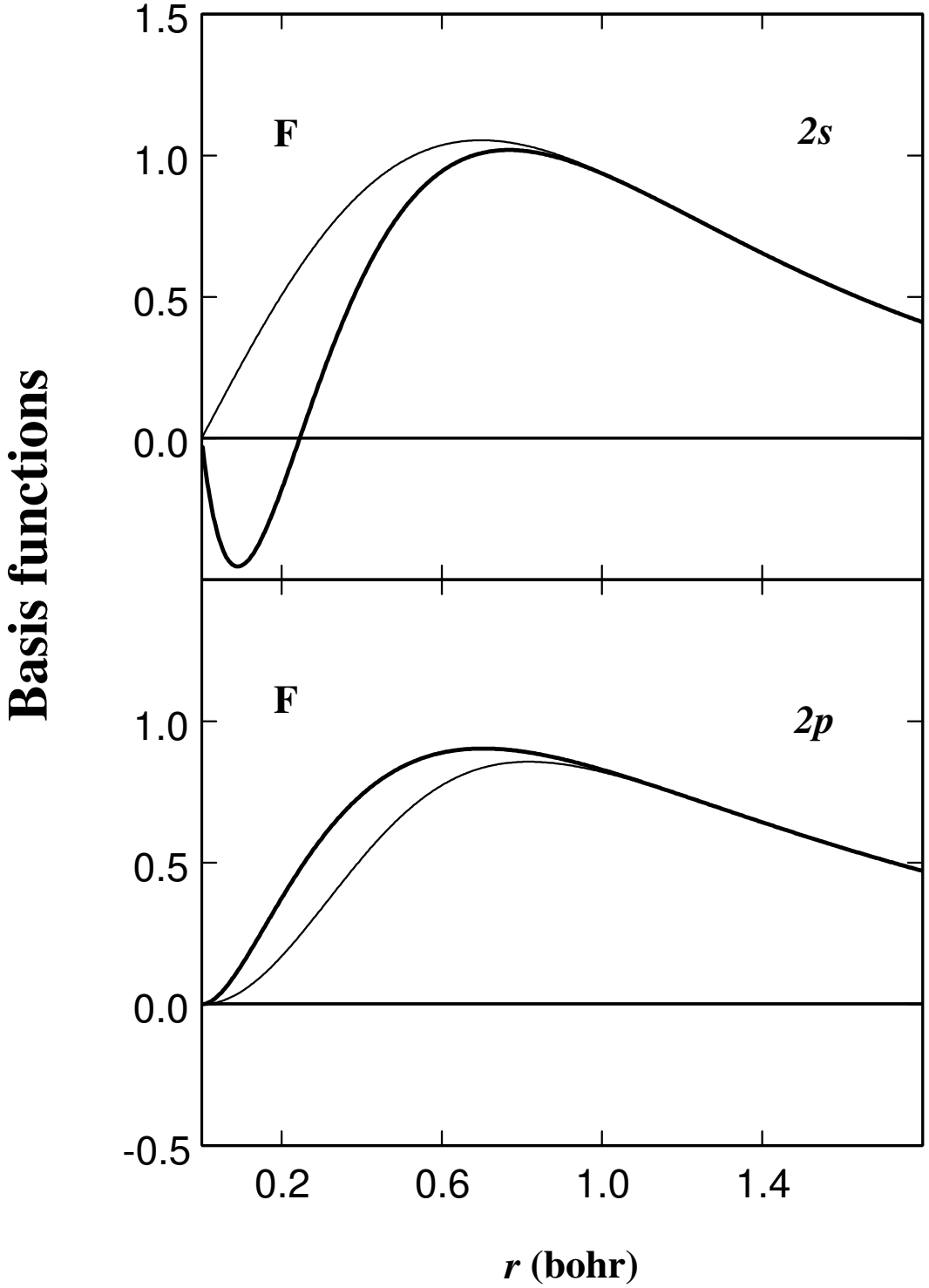


Figure 3: Basis functions for F constructed with $r_c = 1.8$ bohr and $V_0 \equiv 0$, including AE basis functions ($\phi_{2s}$ and $\phi_{2p}$; thick lines) and PS basis functions ($\tilde{\phi}_{2s}$ and $\tilde{\phi}_{2p}$; thin lines).

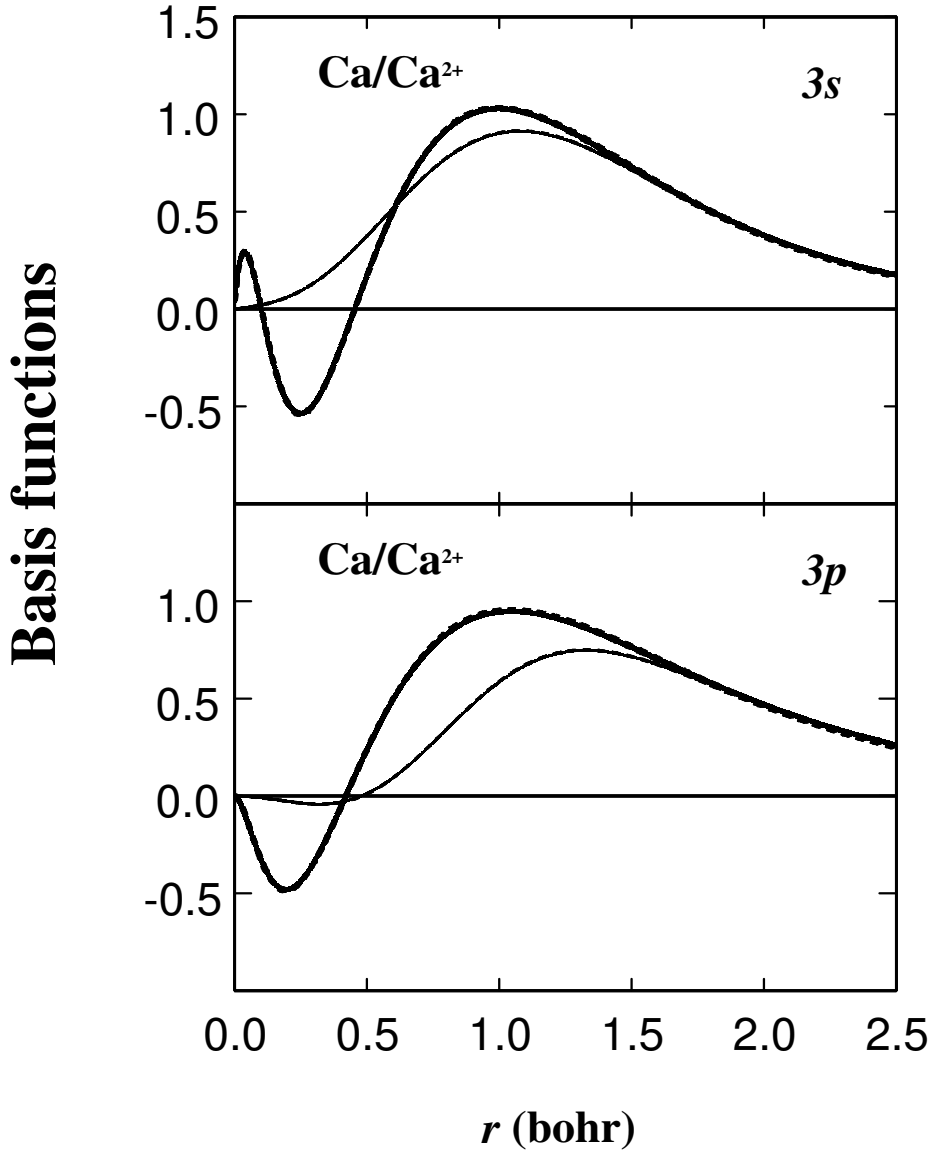


Figure 4: Basis functions for Ca constructed with $r_c = 2.5$ bohr with $V_0 \equiv 0$, including AE basis functions ($\phi_{3s}$ and $\phi_{3p}$; thick lines) and PS basis functions ($\tilde{\phi}_{3s}$ and $\tilde{\phi}_{3p}$; thin lines). Similar functions constructed from the ion $Ca^{2+}$ are plotted with dashed lines, but are barely distinguishable on this scale.

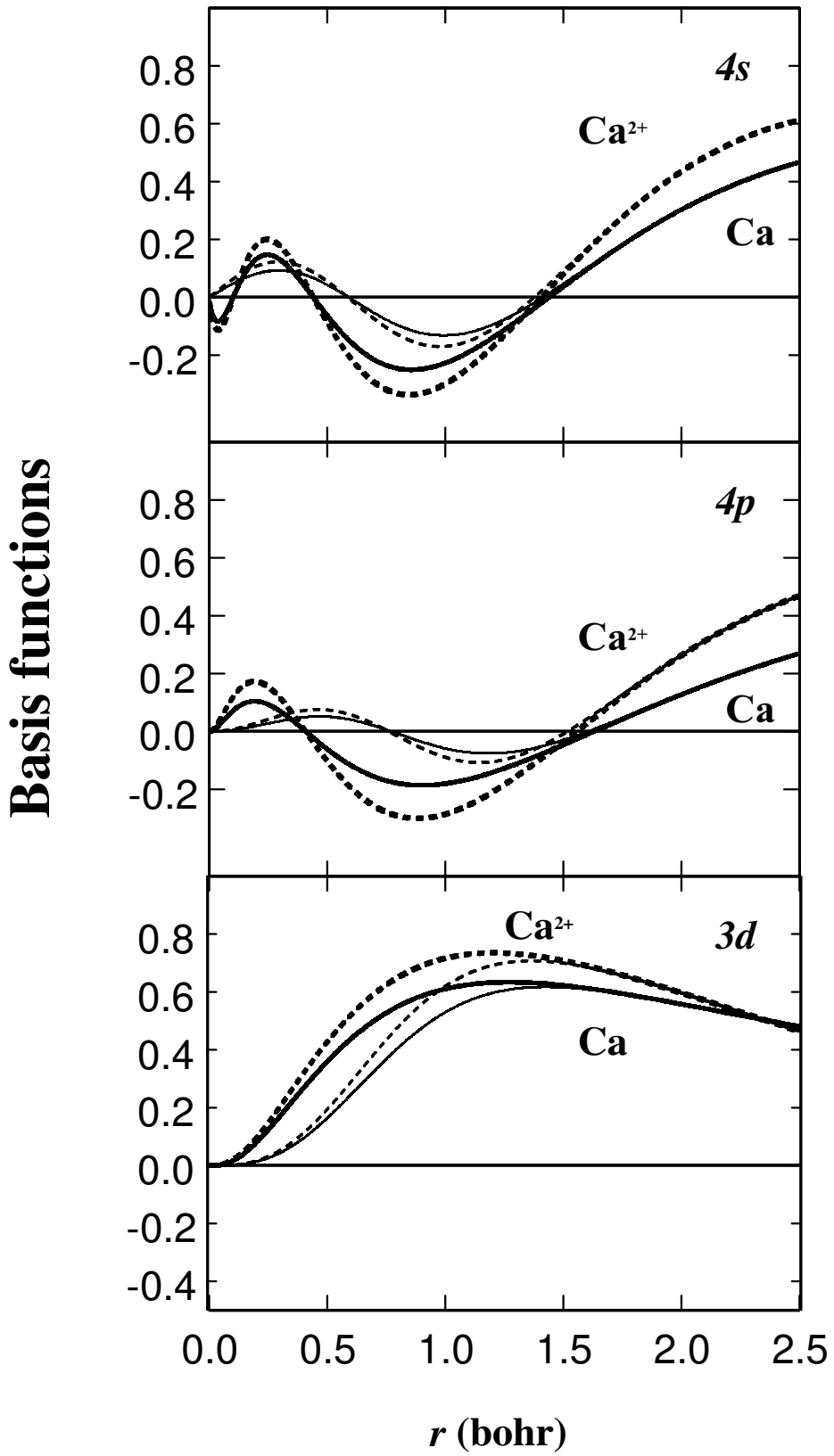


Figure 5: Basis functions for Ca constructed with $r_c = 2.5$ bohr with $V_0 \equiv 0$, including AE basis functions ($\phi_{4s}$, $\phi_{4p}$, and $\phi_{3d}$; thick lines) and PS basis functions ($\tilde{\phi}_{4s}$, $\tilde{\phi}_{4p}$, and $\tilde{\phi}_{3d}$; thin lines). Similar functions constructed from the ion $Ca^{2+}$ are plotted with dashed lines.

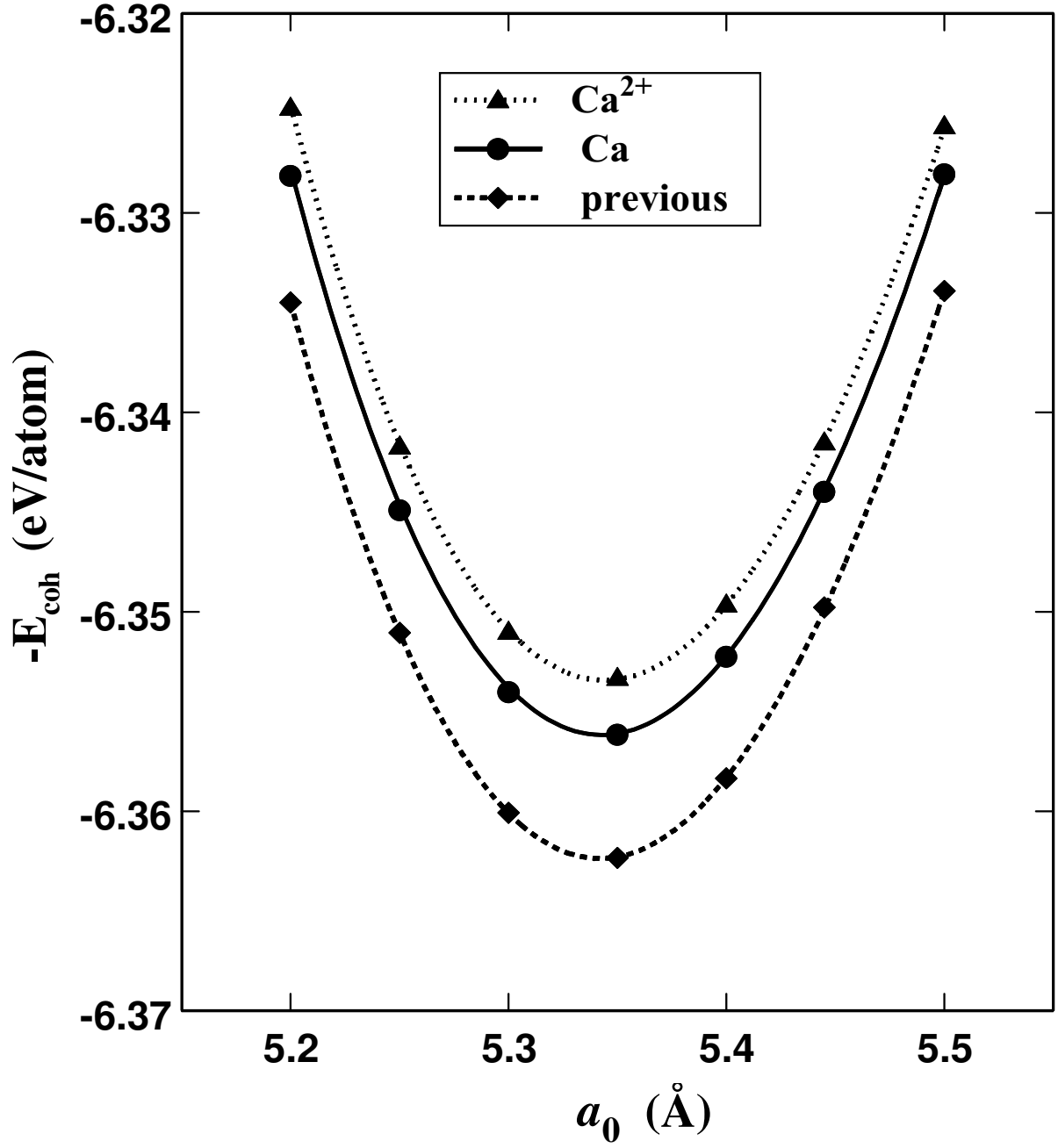


Figure 6: Plot of the negative of the cohesive energy of $CaF_2$ (eV/atom) as a function of cubic lattice constant $a_0$ (Å) obtained from PAW calculations using projectors functions constructed as described in the present work, compared with previous results reported in Ref. (2). The two curves labeled "Ca" and "$Ca^{2+}$" refer to the construction of Ca projectors using neutral and ionic Ca calculations, respectively.

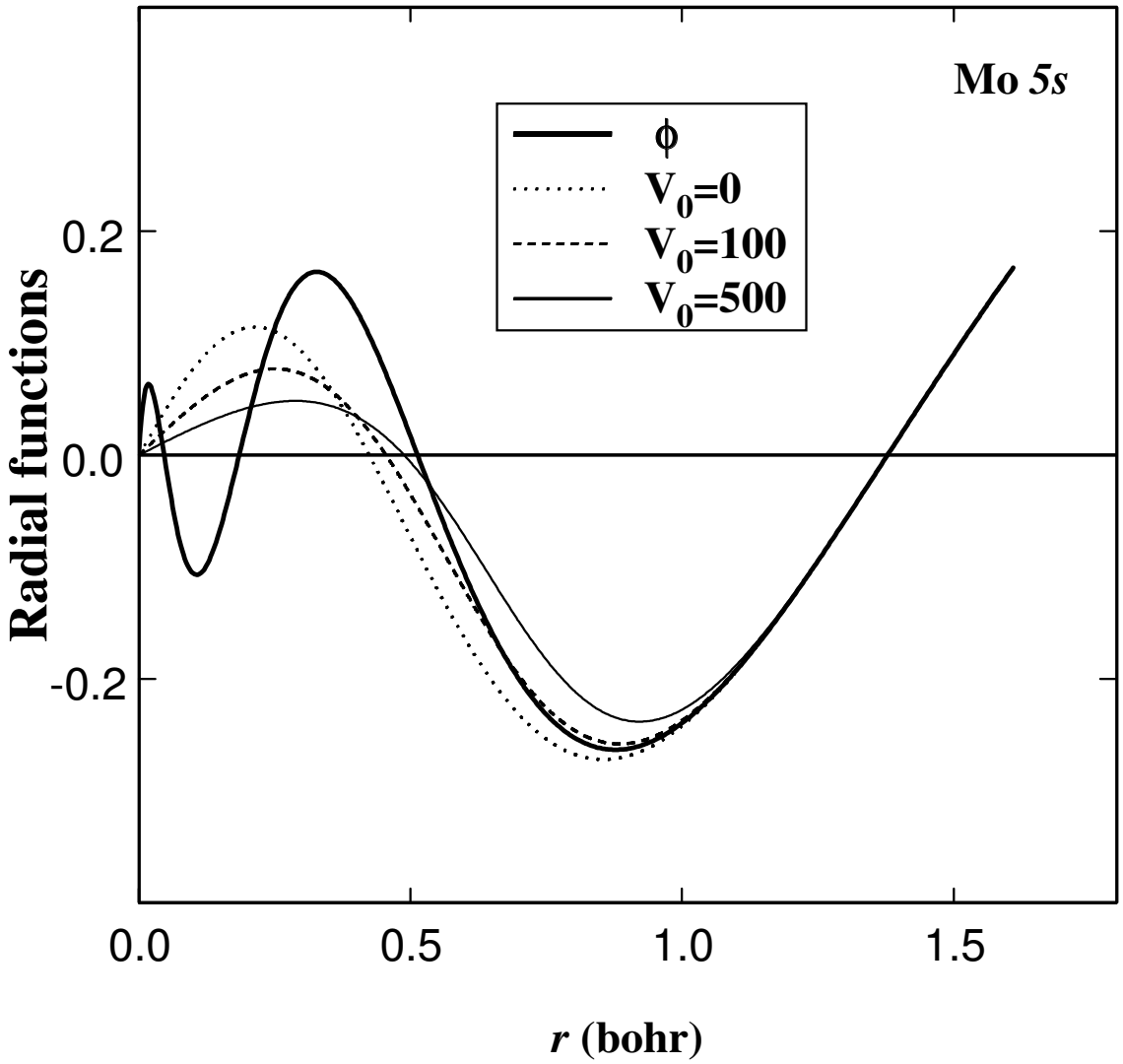


Figure 7: Comparison of PS basis functions for Mo constructed with various values of the local potential amplitude. Plot shows $\tilde{\phi}_{5s}^{Mo}$ constructed using $r_c = 1.6$ bohr and $V_0 = 0, 100$, and 500 Ryd., with the AE function $\phi_{5s}^{Mo}$ included with a thick line for comparison.

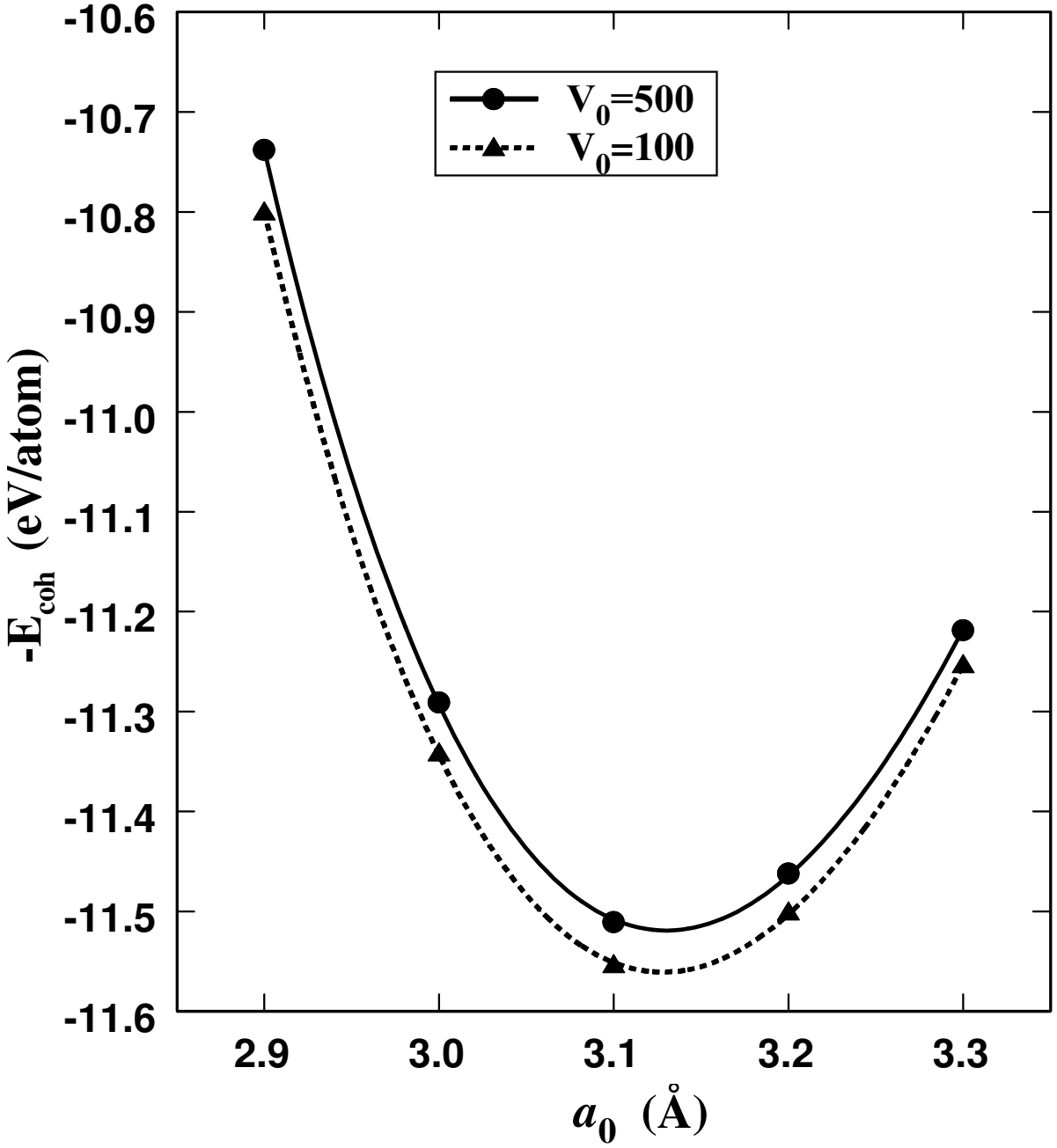


Figure 8: Plot of the negative of the cohesive energy of bcc Mo (eV/atom) as a function of cubic lattice constant $a_0$ (Å) obtained from PAW calculations using projectors functions constructed as described in the present work with Gaussian shaped localized potentials with amplitudes $V_0 = 100$ Ryd. and $V_0 = 500$ Ryd.