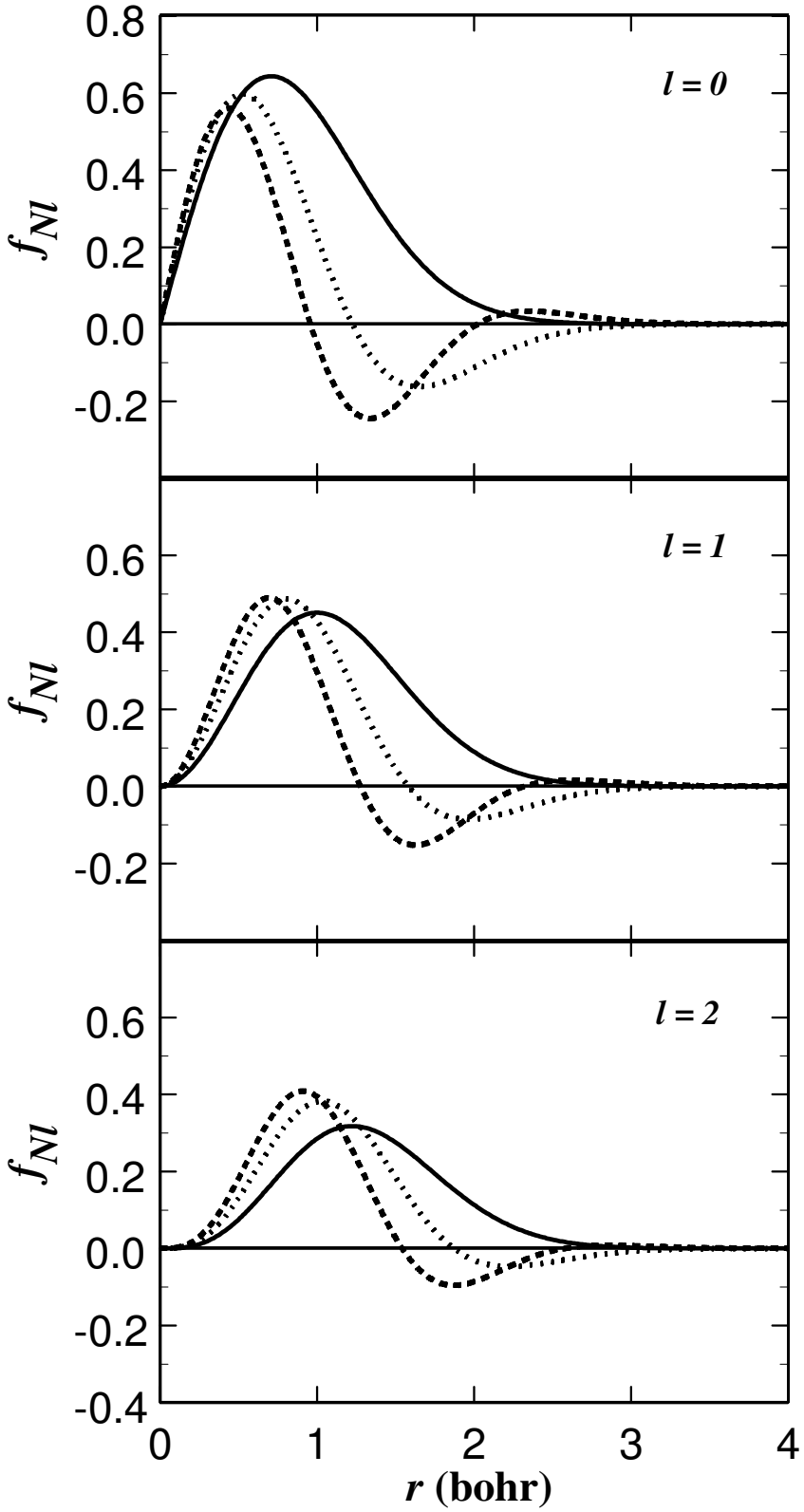

Figure 1: Plots of the projector basis functions defined in Eq. (8) for $\sigma = 1$ and $N = 0$ (solid line), 1 (dashed line), and 2 (dotted line).

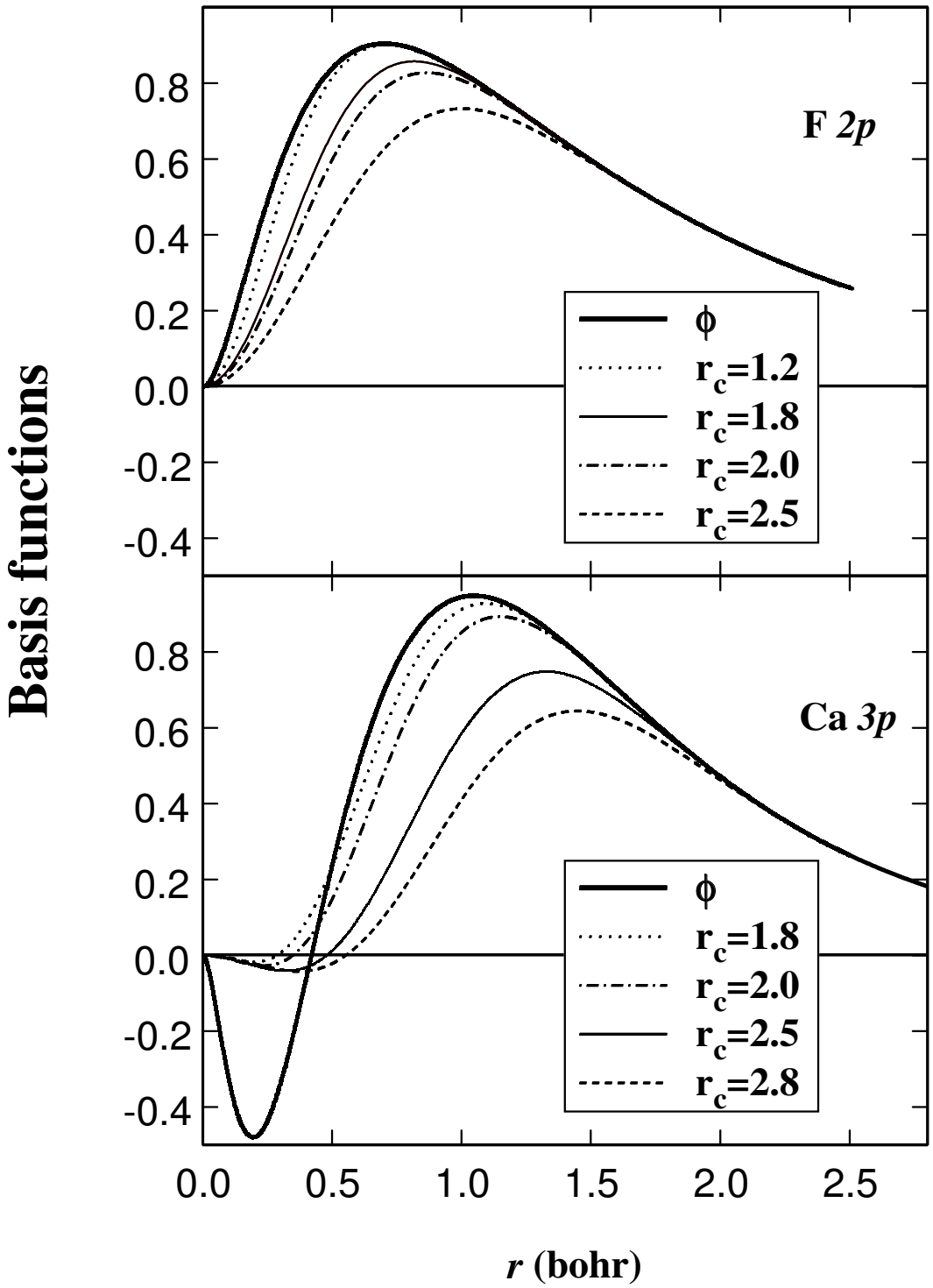

Figure 2: Comparison of PS basis functions constructed with various values of r_c with $V_0 \equiv 0$. Top panel shows F functions $\tilde{\phi}^F_{2p}$ for $r_c = 1.2$, 1.8, 2.0, and 2.5 bohr with the AE function ϕ^F_{2p} included with a thick line for comparison. Bottom panel shows Ca functions $\tilde{\phi}^{Ca}_{3p}$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

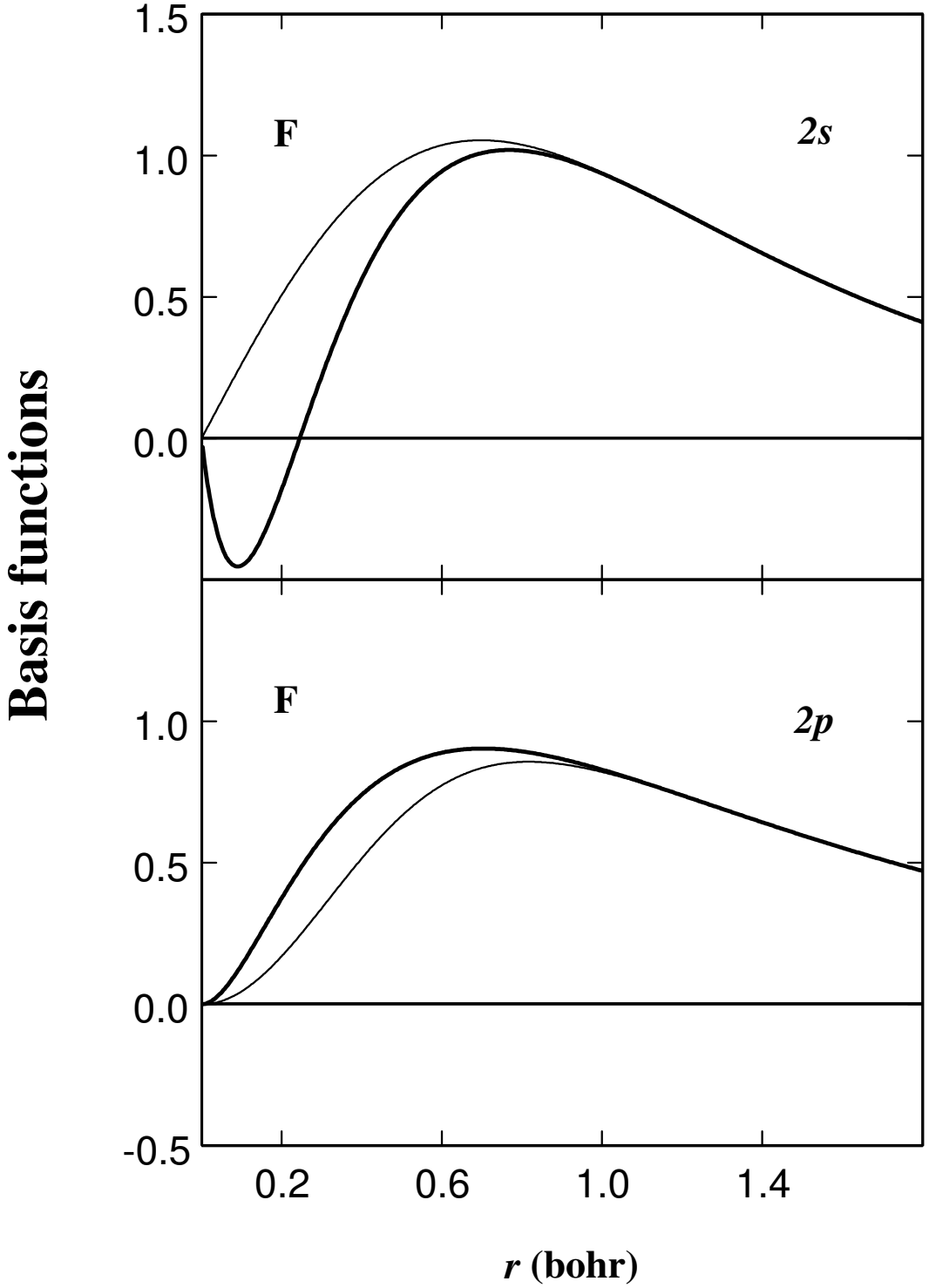

Figure 3: Basis functions for F constructed with $r_c = 1.8$ bohr and $V_0 \equiv 0$, including AE basis functions (ϕ_{2s} and ϕ_{2p}; thick lines) and PS basis functions ($\tilde{\phi}_{2s}$ and $\tilde{\phi}_{2p}$; thin lines).

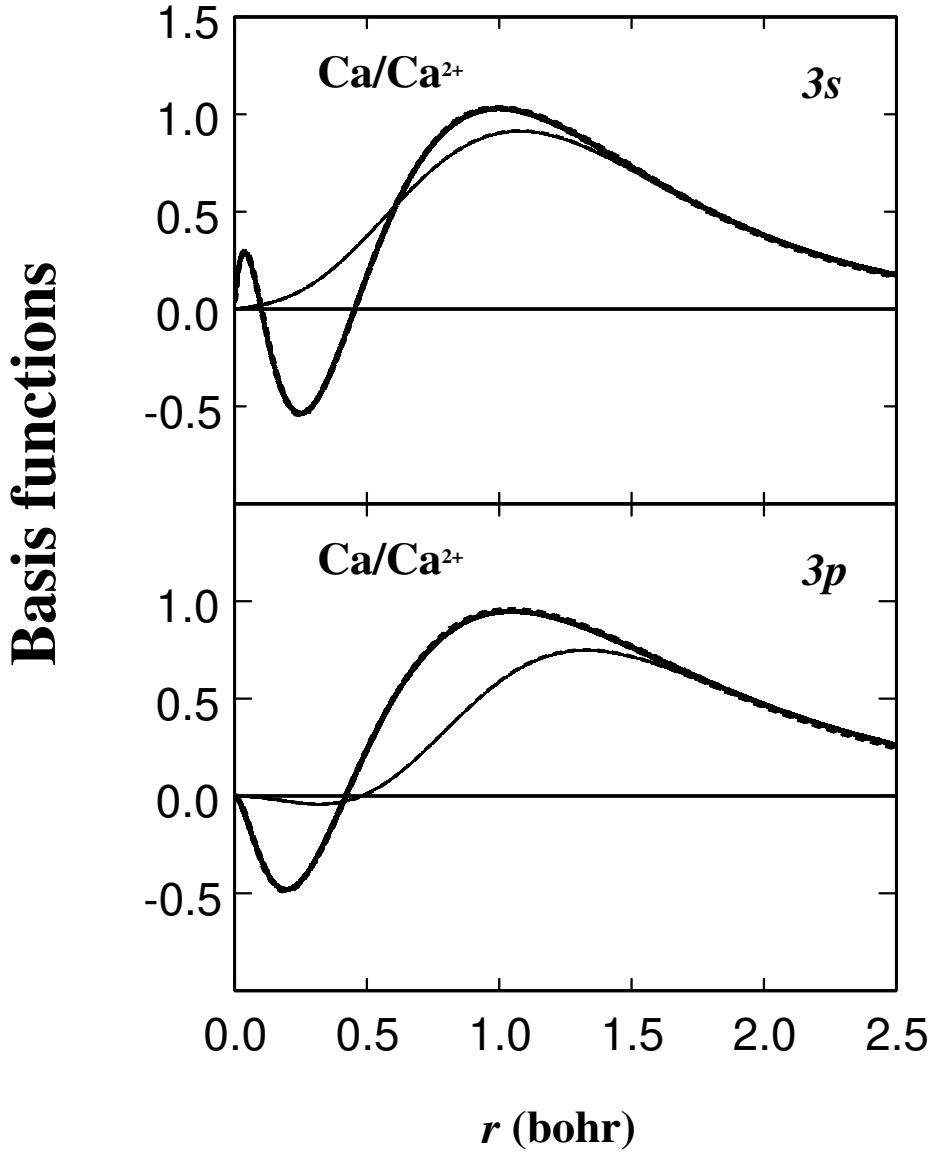

Figure 4: Basis functions for Ca constructed with $r_c = 2.5$ bohr with $V_0 \equiv 0$, including AE basis functions (ϕ_{3s} and ϕ_{3p}; thick lines) and PS basis functions ($\tilde{\phi}_{3s}$ and $\tilde{\phi}_{3p}$; thin lines). Similar functions constructed from the ion Ca^{2+} are plotted with dashed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

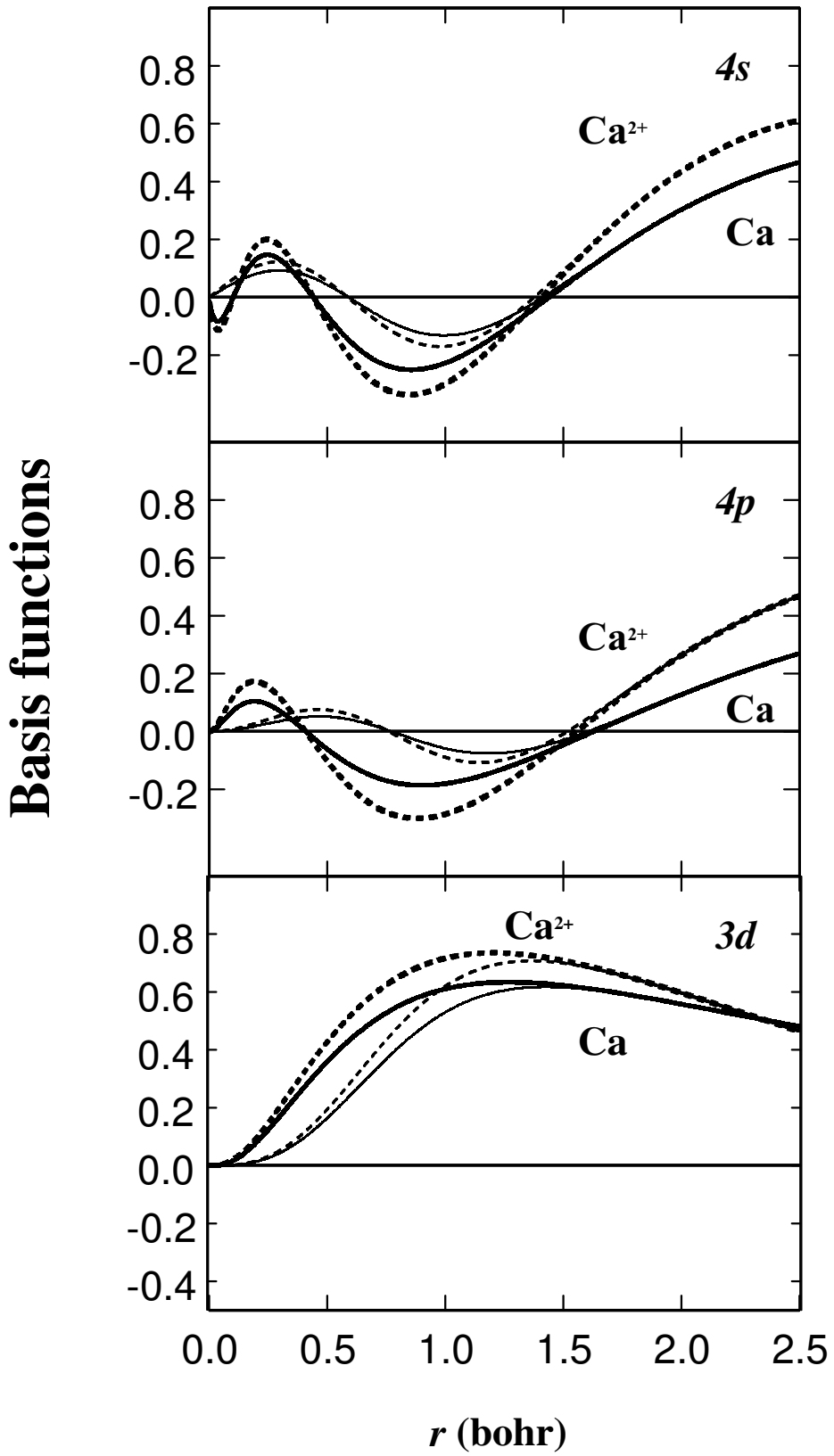

Figure 5: Basis functions for Ca constructed with $r_c = 2.5$ bohr with $V_0 \equiv 0$, including AE basis functions (ϕ_{4s}, ϕ_{4p}, and ϕ_{3d}; thick lines) and PS basis functions ($\tilde{\phi}_{4s}$, $\tilde{\phi}_{4p}$, and $\tilde{\phi}_{3d}$; thin lines). Similar functions constructed from the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

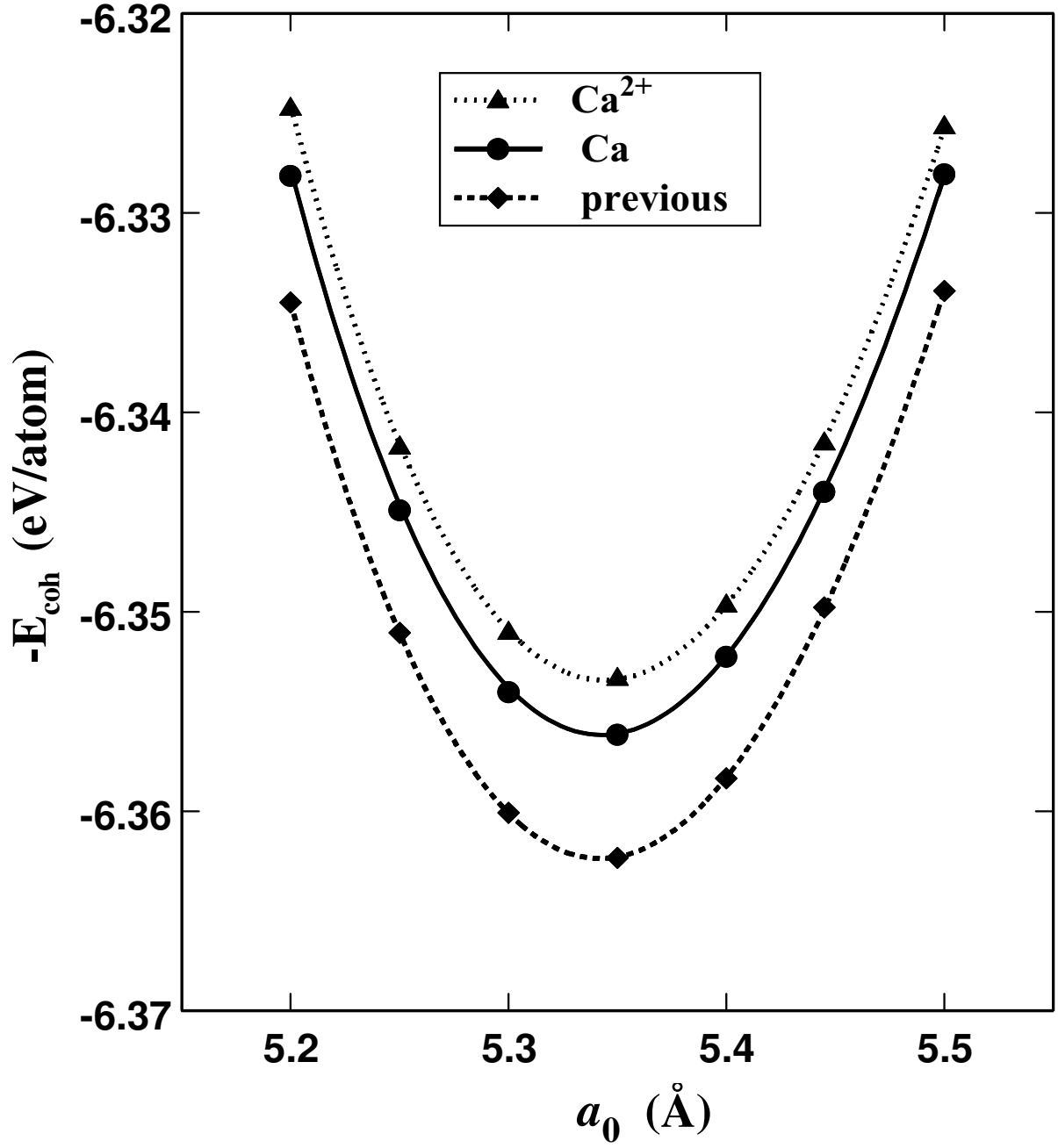

Figure 6: Plot of the negative of the cohesive energy of CaF_2 (eV/atom) as a function of cubic lattice constant a_0 (Å) obtained from PAW calculations using projectors functions constructed as described in the present work, compared with previous results reported in Ref. (2). The two curves labeled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

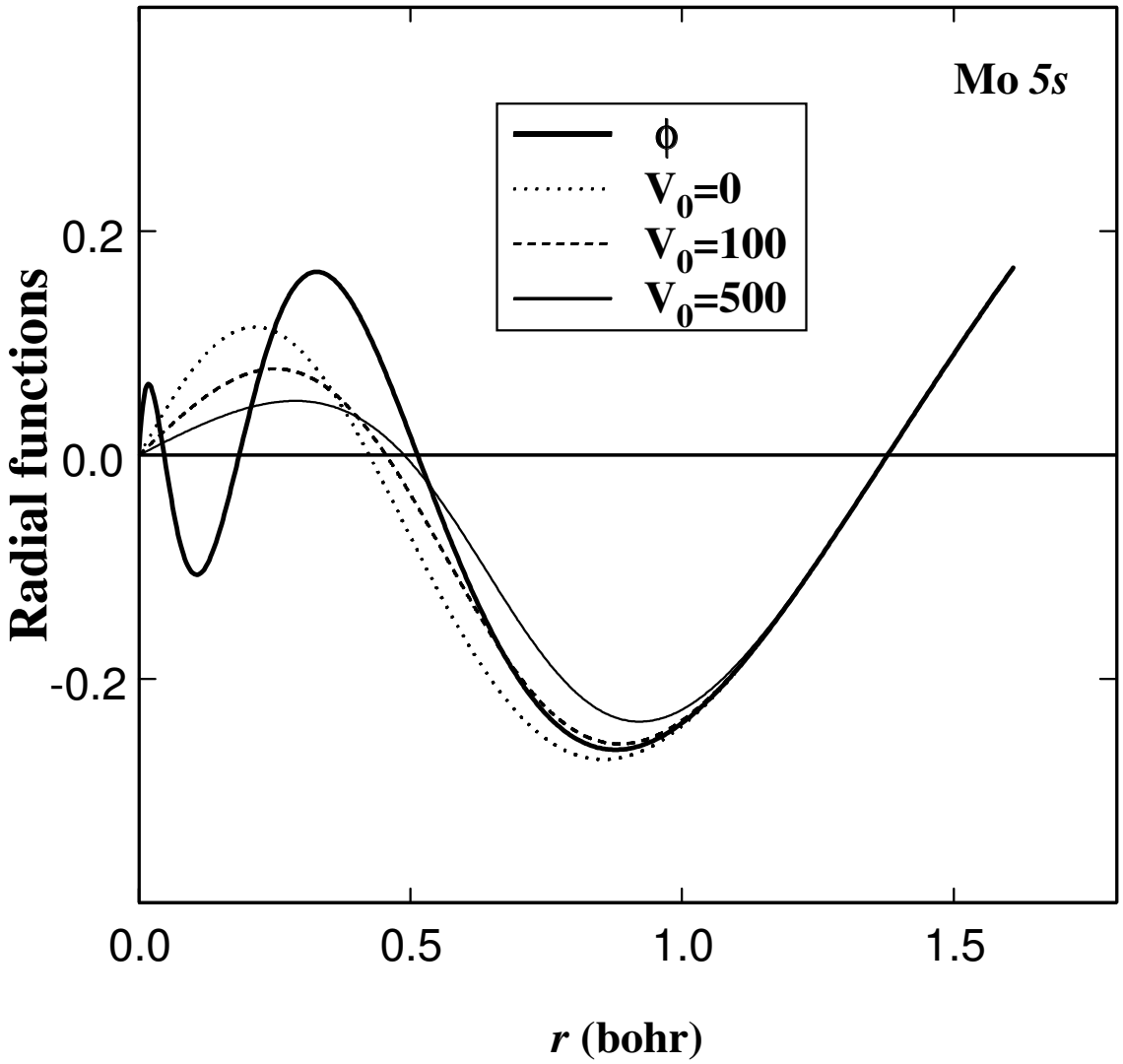

Figure 7: Comparison of PS basis functions for Mo constructed with various values of the local potential amplitude. Plot shows $\tilde{\phi}_{5s}^{Mo}$ constructed using $r_c = 1.6$ bohr and $V_0 = 0, 100$, and 500 Ryd., with the AE function ϕ_{5s}^{Mo} included with a thick line for comparison.

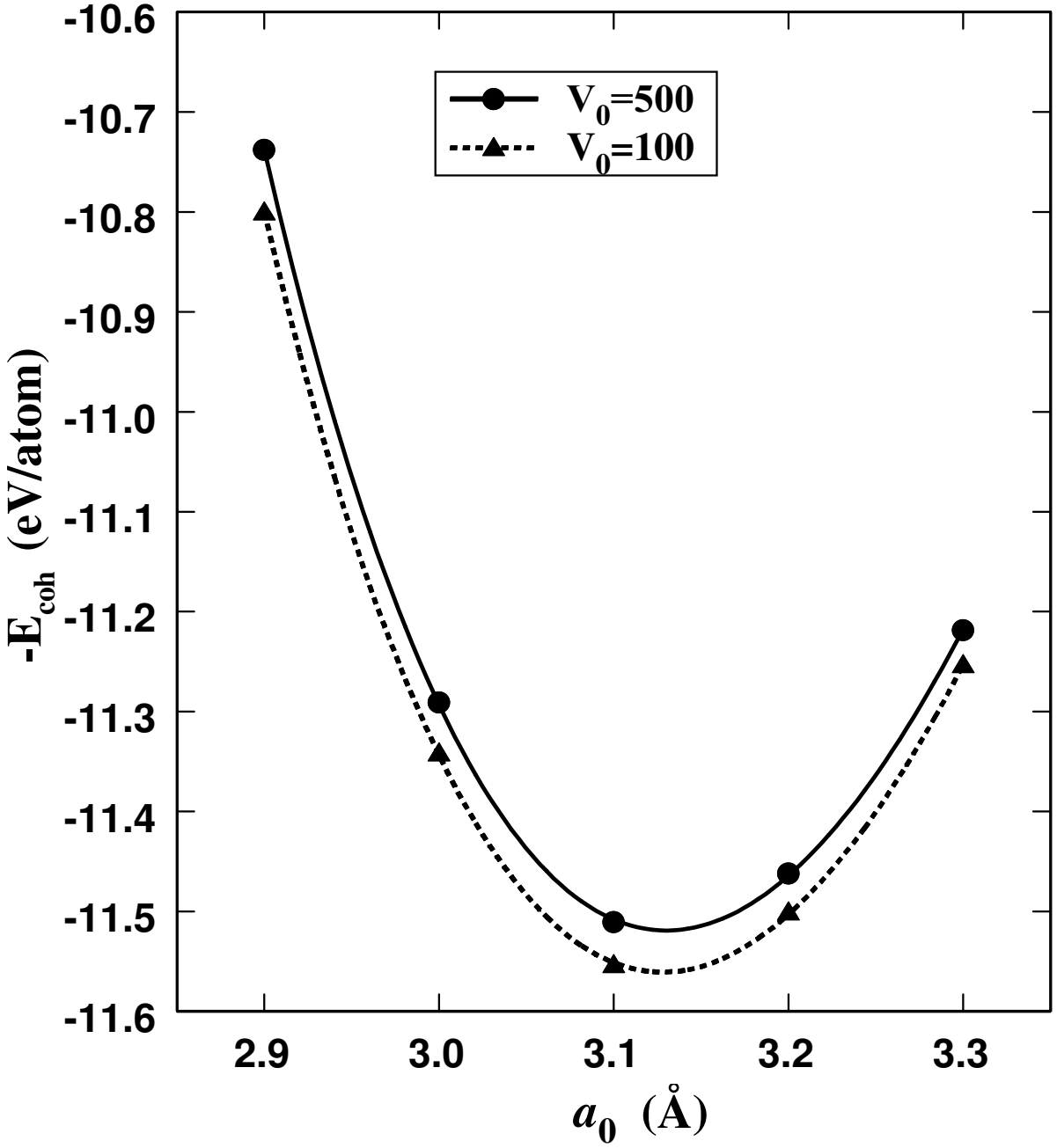

Figure 8: Plot of the negative of the cohesive energy of bcc Mo (eV/atom) as a function of cubic lattice constant a_0 (Å) obtained from PAW calculations using projectors functions constructed as described in the present work with Gaussian shaped localized potentials with amplitudes $V_0 = 100$ Ryd. and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