The electronic structure of CaO may be understood in terms of one valence electron on Ca$^+$ in the field of a -1 point charge and one p-hole on O$^-$, the $\pi$-hole and $\sigma$-hole orientations of which are split by a combination of Pauli repulsion and quadrupole interactions with the Ca$^+$ atomic ion. CaF is an excellent model for the effect of a -1 point charge on Ca$^+$. NaO is an excellent model for the effect of a +1 point charge on O$^-$. This (CaF, NaO) model for CaO accounts for all features of the non-$3\Sigma^+$ states of CaO, including the ordering of electronic states, spin-orbit and lambda-doubling constants, and perturbation matrix elements.

Zn$^+$ differs from Ca$^+$ primarily by a filled and core-like 3d subshell. However, the significantly larger effective nuclear charge seen by the valence orbitals (4s and 4p) of Zn$^+$ causes these orbitals to be much more compact than those on Ca$^+$. The splitting between the lowest lying ZnO $\pi$-hole ($3\Pi$) and $\sigma$-hole ($3\Sigma^+$) states is observed in anion photoelectron spectra and ab initio calculations to be respectively 1.562(12) and 1.3(1) eV, about ten times larger than between the corresponding CaO states. If this larger splitting in ZnO cannot be explained by a simple Rittner-like model, serious doubts would be raised about the validity of the atomic-ions-in-diatomic molecule model, despite its remarkable success for CaO.