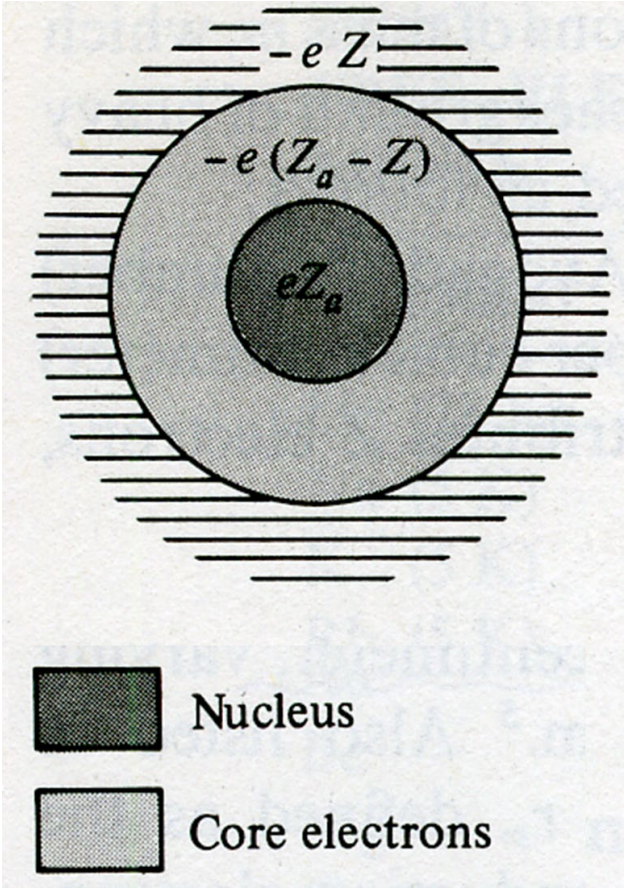
Core electrons are mostly frozen

- Most of the important properties of solid states can be attributed to the valence electrons, while the electrons at the very atomic core remain robustly the atomic states, as it is.
- There might exist a critical radius, usually referred to as the cut-off radius r_{cut} that can materialize the effect of core electrons.



- For example, for carbon atom, we may consider two $(1s)$ electrons are core, and the others are valences. Then, the atomic potential for the FOUR valence electrons,

$$V_{atom}(r) = \begin{cases} -\dfrac{4}{r} & \text{for } r \geq r_{cut} \\ (\ldots) & \text{for } r \leq r_{cut} \end{cases}$$

Pseudopotential

$$V^{PP}(r) = \begin{cases} -\dfrac{4}{r} & \text{for } r \geq r_{cut} \\ (\ldots) & \text{for } r \leq r_{cut} \end{cases}$$

Pseudovalency, Pseudo atomic number Z_{val}

- Very systematic theories have been developed to determine the potential for pseudo-valence electrons (pseudopotential), where the Z_{val} is selected by hands, and r_{cut} can be usually taken shorter than the bond length.

- Norm-conserving type pseudopotential, Ultra-soft type, projected-augmented wave type.

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