First Principles Calculations on the Influence of Solute Elements and Chlorine Adsorption on the Anodic Corrosion Behavior of Mg(0001) Surface

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Highlights

- The influence of solute elements and chlorine adsorption on the anodic behavior of Mg(0001) surface is investigated based on work function change and local electrode potential shift
- Li, Al, Mn, Zn, Fe, Ni, Cu, Y, and Zr are considered as solute atoms in this work
- Cl adsorbate will destabilize Mg atoms on the surface by weakening the metal bonds.
- Strong hybridization between Mg and solute atom orbitals will raise the local electrode potential