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# Adsorption of Arginine, Glycine and Aspartic acid on Mg and Mg-based Alloy Surfaces: A first-principles study

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## Highlights

1. The roles of functional groups for Arg, Gly and Asp in adsorption process are analyzed.
2. Flat configurations with functional groups binding to surfaces are energetically stable.
3. Zn doping promotes the adsorption of Arg, Gly and Asp while Y and Nd doping weaken.
4. Our studies provide basic theoretical foundation for the biomedical coating experiments.

**Abstract:** Studying the adsorption behaviors of biomolecules on the surface of Mg and Mg-based alloy has a fundamental and important role for related applications in biotechnology. In the present work, we systematically investigate and compare the adsorption properties of three typical amino acids, i.e., Arg (arginine), Gly (glycine) and Asp (aspartic acid), which form RGD tripeptide, on the Mg (0001) surface with various doping (Zn, Y, and Nd), and aim to realize proper binding between biomolecules and Mg and Mg-based biomedical materials. Our results show that flat adsorption configurations of the functional

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