中国腐蚀与防护学报 >>2011 >>31 >>(6)

中国腐蚀与防护学报 2011, **31**(6) 478-482 **DOI**: **ISSN**: 1005-4537 **CN**: 31-1421/TG

研究报告

5种氨基酸对铁缓蚀机理的分子动力学模拟

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摘要： 用分子动力学方法模拟计算了甘氨酸、亮氨酸、天冬氨酸、精氨酸及蛋氨酸5种氨基酸类缓蚀剂与Fe(100)晶面、(110)晶面及(111)晶面在酸性条件下的相互作用。结果发现，5种氨基酸与Fe的3个晶面结合能的排列顺序由小到大均为甘氨酸<亮氨酸<天冬氨酸<精氨酸<蛋氨酸；同一氨基酸分子与Fe(111)晶面结合能最大，与Fe(110)晶面结合能次之，与Fe(100)晶面结合能最小。对体系各种相互作用以及对关联函数g(r)的分析表明，结合能主要由库仑相互作用能和范德华能提供。金属Fe原子与氨基酸中的N、 O及S原子形成了配位键，与Fe晶面结合的氨基酸分子构型发生扭曲变形，但形变能均远小于相应的非键相互作用能。

关键词： 氨基酸 铁 缓蚀机理 分子动力学 对关联函数

MOLECULAR DYNAMICS SIMULATION OF CORROSION INHIBITING MECHANISM OF IRON BY FIVE KINDS OF AMINO ACIDS

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Abstract: The interactions between five kinds of amino acid corrosion inhibitors, i.e. glycin、leucine、aspartic acid、arginine and methionine and (100), (110), (111) crystal surfaces of Fe have been simulated by molecular dynamics. The results show that the orders of binding energy for five kinds of amino acids with three Fe crystal surfaces are as follows: glycin<leucine<aspartic acid<arginine<methionine, and for the same amino acid, the binding energy of amino acid with (111) crystal surface is the largest, and that with (100) crystal surface is the least. The analysis of various interactions and pair correlation functions g(r) of all systems indicates that binding energies are mainly provided by coulomb interaction energy and Van der Waals energy. Coordination bonds are formed between the metal iron atoms and the nitrogen、oxygen and sulfur atoms in amino acids. The configurations of amino acids have been deformed during their combining with Fe crystal surfaces, but the deformation energies of amino acids are far less than respective nonbonding energies.

Keywords: amino acid iron corrosion inhibition mechanism molecular dynamics pair correlation functions

收稿日期 2011-03-22 **修回日期** 2011-05-04 **网络版发布日期** 2011-12-14

DOI:

基金项目:

国家自然科学基金项目(20906052)，江苏科技支撑计划(BE2011835)，南京理工大学自主科研专项(2011-YBX65)，

盐城工学院开放项目(XKY2011004)和盐城工学院应用基础研究项目(XKR2011005)资助

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