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研究论文

多氨基多醚基亚甲基膦酸的合成及其阻垢机理的**MD**模拟

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摘要 以端氨基聚醚、亚磷酸、甲醛、浓盐酸等为原料合成了新型水处理剂多氨基多醚基亚甲基膦酸(PAPEMP), 并通过红外、核磁等手段对产品进行了表征. 采用分子动力学(MD)模拟退火方法, 研究了周期性边界条件下PAPEMP与方解石晶体的相互作用, 探讨了该相互作用的本质, 并初步阐释了PAPEMP的阻垢机理. 结果发现, PAPEMP分子(n＝1～8)与方解石 晶面的结合能强弱排序依次为(按聚合度) 5＞6＞4＞3＞8＞2＞7＞1. 对体系各种相互作用以及对关联函数$g(r)$的分析表明, 超分子体系的结合能主要由库仑作用(包括离子键)提供, 并含少量氢键成分; van der Waals作用为正值, 不利于结合体系的形成. 能量分析表明, 与方解石晶面结合的PAPEMP (n＝1～8)分子均发生了明显的扭曲变形.

关键词 多氨基多醚基亚甲基膦酸 分子动力学 方解石 阻垢机理 结合能 对关联函数 形变能

分类号

Synthesis and Molecular Dynamics Simulation of Anti-scaling Mechanism for Polyether Polyamino Methylene Phosphonates

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Abstract Polyether polyamino methylene phosphonates (PAPEMP), a new type of reagent for water treatment, was synthesized from polyoxypropylene-diamine, phosphorous acid, formaldehyde and concentrated hydrochloric acid. The product was characterized by IR and NMR. The interactions between PAPEMP and calcite crystal were studied by means of simulated annealing molecular dynamics technique with period boundary condition. The essence of such interactions and scale inhibition mechanism of PAPEMP were also discussed tentatively. Results showed that the order of binding energies for PAPEMP (n＝1～8) with crystal surface of calcite was as follows: 5＞6＞4＞3＞8＞2＞7＞1, according to repeated units. The analysis on various interactions and pair correlation functions of all systems indicated that binding energies were mainly provided by coulomb interaction including electrovalent bond, and a little came from hydrogen bond, while van der Waals interaction was against the formation of combined systems on account of its positive value. From the energy analysis results, PAPEMP (n＝1～8) molecules could be conclusively deformed severely when they were combined with calcite crystal surface.

Key words polyether polyamino methylene phosphonates molecular dynamics calcite scale inhibition mechanism binding energy pair correlation function deformation energy

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