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论文

缓蚀剂膜抑制腐蚀介质扩散行为的分子动力学模拟

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摘要:

采用分子动力学模拟方法研究了4种腐蚀介质粒子(H_2O, H_3O^+, HS^-和Cl^-)在6种不同烷基链长的1-(2-羟乙基)-2-烷基-咪唑啉缓蚀剂膜中的扩散行为. 计算了腐蚀介质粒子在不同缓蚀剂膜中的扩散系数、膜的自由体积分数、粒子与膜的相互作用能等, 并对缓蚀剂膜抑制腐蚀介质粒子扩散行为的微观机理进行了分析. 计算结果表明, 6种缓蚀剂膜均可有效阻碍腐蚀介质粒子向金属表面的扩散, 从而达到抑制或延缓腐蚀的目的; 随烷基链长的增加, 缓蚀剂膜对腐蚀介质粒子扩散行为的抑制能力逐渐增强; 同种缓蚀剂膜对正负离子H_3O^+, HS^-和Cl^-比对中性的H_2O分子具有更强的扩散抑制能力.

关键词: 腐蚀介质; 缓蚀剂膜; 扩散; 分子动力学模拟

Molecular Dynamics Simulation of the Corrosive Medium Diffusion Behavior Inhibited by the Corrosion Inhibitor Membranes

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Abstract:

The diffusion behavior of four corrosive media(H_2O, H_3O^+, HS^-, and Cl^-) in membranes formed by six 1-(2-hydroxyehtyl)-2-alkyl-imidazoline compounds with various alkyl chain lengths was investigated with molecular dynamics(MD) simulation. The simulation was performed by calculation of diffusion coefficients of corrosive particles in the membranes, fractional free volumes of the membranes, and the interaction energies between particles and membranes. And the microscopic inhibition mechanism of the membranes for diffusion of corrosive particles was explored. The calculated results showed that all the membranes formed by corrosion inhibitor molecules can effectively prevent the corrosive particles from diffusing to the metal surface, and thus inhibit or delay the corrosion process. With the elongation of alkyl chain length, the inhibitor membranes showed increased capacity for prevention of diffusion of corrosive particles. While membranes formed by identical molecules showed more preferable inhibition performance for cations and anions(H_3O^+, HS^-, and Cl^-) than that for neutral molecule(H2O).

Keywords: Corrosive medium; Corrosion inhibitor membrane; Diffusion; Molecular dynamics simulation

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参考文献:

[1]ZHANG Jun(张军), HU Song-Qing(胡松青), WANG Yong(王勇), et al.. Acta Chim. Sinica(化学学报)[J], 2008, 66(22): 2469—2475

[2]ZHANG Shu-Guang(张曙光), CHEN Yu(陈瑜), WANG Feng-Yun(王风云). Acta Chim. Sinica(化学学报)[J], 2007, 65(20): 2235—2242

[3]LIU Dan(刘丹), ZHANG Xiao-Tong(张晓彤), GUI Jian-Zhou(桂建舟), et al.. J. Petrochem. Univ.(石油化

工高等学校学报)[J], 2004, 17(3): 9—13
[4]SHI Jian(石剑), ZHANG Min-Hua(张敏华), DONG Xiu-Qin(董秀芹). Chem. J. Chinese Universities(高等学校化学学报)[J], 2007, 28(3): 518—521
[5]LIU Qing-Zhi(刘清芝), YANG Deng-Feng(杨登峰), HU Yang-Dong(胡仰栋). Chem. J. Chinese Universities(高等学校化学学报)[J], 2009, 30(3): 568—572
[6]HE Yan(何岩), ZHANG Min-Hua(张敏华), JIANG Hao-Xi(姜浩锡). Chem. Ind. Eng(化学工业与工程)[J], 2009, 24(1): 57—61
[7]Yang J. Z., Chen Y., Zhu A. M.. J. Membrane. Sci.[J], 2008, 318(2): 327—333
[8]Hofmann D., Fritz L., Ulbrich J., et al.. Computational and Theoretical Polymer Science[J], 2000, 10(5): 419—436
[9]Sylvie N., David B.. Macromolecules[J], 2008, 41(7): 2711—2721
[10]Luis S. Z. R., Estrada A., Benavides A., et al.. J. Mex. Chem. Soc.[J], 2002, 46(4): 335—340
[11]Accelrys Materials Studio, Version 4.1.0.0[CP], San Diego: Accelrys Software Inc., 2006
[12]Sun H., Ren P., Fried J. R.. Computational and Theoretical Polymer Science[J], 1998, 8(1/2): 229—246
[13]Andrea T. A., Swope W. C., Andersen H. C.. J. Chem. Phys.[J], 1983, 79(4): 4576—4584
[14]Berendsen H. J. C., Postma J. P. M., Funsteren W. F.. J. Chem. Phys.[J], 1984, 81(4): 3684—3690
[15]Prathab B., Aminabhavi T. M., Parthasarathi R.. Polymer[J], 2006, 47(19): 6914—6924
[16]Yang H., Liu Y., Zhang H., et al.. Polymer[J], 2006, 47(21): 7607—7610
[17]Lin Y. C., Xu C.. Chem. Phys. Lett.[J]. 2005, 412(4): 322—326
[18]Zhang Q. G., Liu Q. L., Chen Y., et al.. Chem. Eng. Sci.[J], 2009, 64(1): 334—340
[19]Zhou J. H., Zhu R. X., Zhou J. M., et al.. Polymer[J], 2006, 47(14): 5206—5212
[20]Pan F. S., Peng F. B., Jiang Z. Y.. Chem. Eng. Sci.[J], 2007, 62(3): 703—710
[21]Babu C. S., Lim C.. Chem. Phys. Lett.[J], 1999, 310(1/2): 225—228
[22]Arnau C., Olle E., Juan J. P.. J. Phys. Chem. B[J], 2008, 112(7): 1397—1408
[23]Lehmann A., Konig G., Rieder K. H.. Phys. Rev. Lett.[J], 1994, 73(23): 3125—3128
[24]Pan F. S., Peng F. B., Lu L. Y., et al.. Chem. Eng. Sci.[J], 2008, 63(4): 1072—1080

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