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键合剂对HTPB与Al/Al2O3之间界面作用的分子模拟

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Title: Molecular Simulation of Effect of Bonding Agents on Interface Interaction for HTPB and Al/Al2O3

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关键词: 物理化学; 端羟基聚丁二烯; 键合剂; 固体推进剂; 分子模拟; 力学性能

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摘要: 采用分子动力学(MD)方法和COMPASS力场，研究了键合剂对丁羟推进剂中端羟基聚丁二烯(HTPB)与Al/Al2O3之间界面的吸附能与力学性能。结果表明，键合剂在Al2O3晶面的吸附能高于HTPB在Al2O3晶面的吸附能，而在Al晶面的规律并不明显。键合剂(TEA)与HTPB在Al2O3晶面吸附能远高于在Al晶面，Al2O3晶体(010)晶面高于 (001)晶面，Al晶体(001)晶面高于(011)晶面。两晶面中吸附能愈高，力学性能愈好。几种键合剂对吸附体系力学性能(弹性模量)的作用次序：TAZ＞TEA＞MAPO·HAC＞MAPO＞HX752。

Abstract: The molecular dynamics method and COMPASS force field were adopted to simulate adsorption energy and mechanical properties of the interfaces constructed by HTPB, bonding agents and crystal faces of Al and Al2O3. The results show that the adsorption energy of bonding agents on Al2O3 crystal is more than that of HTPB on Al2O3 crystal, while the adsorption rule on Al crystal is not distinct. The adsorption energy of bonding agent(TEA) and HTPB on Al2O3 crystal faces is far more than that on Al crystal faces. The (001) surface of Al has the greater adsorption energy than that of (011) surface, while the (010) surface of Al2O3 has the greater adsorption energy than that of (001) surface.The higher the adsorption energy, the better the mechanical property. The effect of

bonding agents on mechanical properties (tensile modulus) of adsorption system decreases in the order: TAZ>TEA>MAPO·HAC>MAPO>HX 752.

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