

Accepted Manuscript

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PII: S0009-2614(15)00847-7
DOI: <http://dx.doi.org/doi:10.1016/j.cplett.2015.11.006>
Reference: CPLETT 33409

To appear in:

Received date: 17-8-2015
Revised date: 3-11-2015
Accepted date: 5-11-2015

Please cite this article as: L. Yan, Y. Yang, H. Jiang, B. Zhang, H. Zhang, The adsorption of methyl methacrylate and vinyl acetate polymers on α -quartz surface: a molecular dynamics study, *Chem. Phys. Lett.* (2015), <http://dx.doi.org/10.1016/j.cplett.2015.11.006>

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The adsorption of methyl methacrylate and vinyl acetate polymers on α -quartz surface: a molecular dynamics study

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Highlight

1. molecular dynamics simulation was performed to investigate the interface between two polymers (PVA, PMMA) and α -quartz.
2. both the polymers can be adsorbed onto the quartz surface, forming hydrogen bonds and the carbonyl groups in the polymer molecules play a crucial role in the interaction between polymer and quartz.
3. There was no significant difference between the adsorption energies for the two polymers on quartz surface, but there were more hydrogen bonds formed in PVA/quartz surface than PMMA.

Abstract:

The molecular dynamics simulation was used to investigate the adsorption of polymethyl methacrylate (PMMA) and polyvinyl acetate (PVA), the commonly used surface coating materials, on α -quartz surface. The objective is to understand the interactions between quartz surface and polymers. The results clearly show adsorption of both polymers onto the quartz surface. Carbonyl group plays a significant role in the adsorption process. The adsorption energies of PMMA and PVA on α -quartz surface did not show significant difference, however, more hydrogen bonds were observed on the PVA/quartz system than PMMA/quartz. These observations might offer some insights on the polymer-quartz adhesion and its failure mechanism.

Keywords: Molecular dynamic simulation; polymethyl methacrylate; polyvinyl acetate; quartz adsorption

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