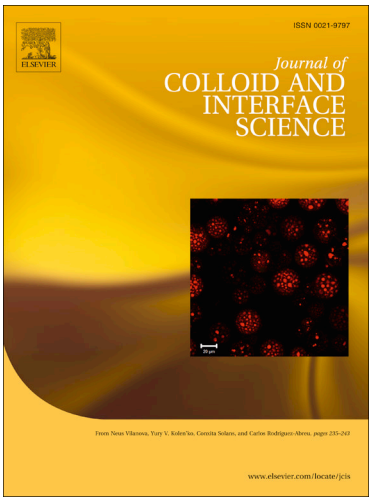

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Nanosilica modified by polydimethylsiloxane depolymerized and chemically bound to nanoparticles or physically bound to unmodified or modified surfaces: Structure and interfacial phenomena

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Abstract

Three polydimethylsiloxanes (PDMS200, PDMS1000, and PDMS12500 with numbers showing the viscosity values dependent on the molecular weight) were used for adsorption (14-95 wt.% PDMS) onto unmodified and PDMS-modified (16.7 wt.% PDMS using dimethyl carbonate (DMC) as a siloxane bond breaking reagent) nanosilica A-300. The materials were studied using microscopy, infrared spectroscopy, thermodesorption, calorimetry, ethanol and water/ethanol evaporation, nitrogen adsorption-desorption, and quantum chemical methods. The interfacial and temperature behaviors of a PDMS layer at a silica surface depend strongly on the type of bonding to silica particles, molecular weight and content of PDMS. Upon chemical bonding, shorter PDMS200 forms a denser coverage of the silica surface since S_{BET} diminution is larger and residual free silanols are practically absent (the degree of free silanol substitution $\Theta > 0.95$) in contrast to the reactions with PDMS1000/DMC or PDMS12500/DMC providing $\Theta = 0.60$-0.63 at larger S_{BET} values. Upon thermal decomposition of the PDMS layer, oxidation/depolymerization desorption gives a greater contribution than pure depolymerization destruction. An increase in the PDMS adsorption layer thickness leads to enhancement of the depolymerization contribution because the oxidation mainly occurs at the top of the layer, but the depolymerization can occur in the total PDMS layer. The adsorption, desorption, and evaporation processes of low-molecular weight probes at a surface of PDMS-modified nanosilica depend strongly on the type of bonding and content of PDMS. Thus, the most effective hydrophobization of nanosilica by PDMS/DMC could be carried out using the shortest polymer giving the shortest PDMS fragments upon the interaction with DMC that is of interest from a practical point of view.

Keywords: Polydimethylsiloxane adsorption; Hydrophobized nanosilica; Textural characteristics; Thermal oxidation; Depolymerization; Ethanol evaporation

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