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Energy mapping and surface energy heterogeneity profiles of surface-modified carbon nanotubes using IGC-SEA technique

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Statement of the Problem: Carbon nanotubes are promising support for Co/Mo-catalyst used in production of fuel-components of high hydrogen/carbon ratio in hydrocracking and reinforcing constituent for nanocomposites. To avoid agglomeration in a supported nanoparticulate catalyst or nanocomposites, the CNT surfaces are often exposed to modification processes using poly-functional coupling agents. The quantitative characterization of the effectiveness of surface treatments by surface energy mapping is of high importance.

Methodology & Theoretical Orientation: Inverse gas chromatography (IGC) was used for surface energy analysis, which supplies information on surface characteristics of the nanoparticles. Experimental results obtained by a Surface Energy Analyzer (SEA) for untreated and olefin maleic-anhydride copolymer treated carbon nanotubes are presented. The effectiveness of surface treatments was quantified in terms of dispersive and specific surface energies, and of the acid-base parameters of the CNT surfaces. Furthermore, the surface energy heterogeneity profiles and distributions of the CNTs were determined by a unique energy mapping.

Conclusion & Significance: The surface energy mapping of the CNT samples indicated that the dispersive and specific components of surface energy of untreated CNT sample are quasi-constant in the region of low surface coverage. The relatively high values of dispersive surface energy can be attributed to a large nonpolar interaction potential of CNT, which explains its high agglomeration tendency. However, the surface energy heterogeneity profiles of the treated CNTs prove that both the dispersive and the specific parts of surface energy of the copolymer modified CNT surface are slightly non-homogenous in the region of low surface coverage. The quantitative surface energy analysis obtained by IGC/SEA methodology demonstrated that surface treatments of CNTs resulted in significant changes of surface energies: the dispersive component of surface energies of the CNTs decreased by 60% and the specific surface energy of CNT surfaces increased more than threefold.

Biography

András Dallos has expertise in "Experimental and computational physical chemistry: Measurement and modeling of bulk and surface properties of pure compounds, mixtures, macromolecules, nanomaterials and composites". His research activities focus on the inverse gas chromatographic and calorimetric determination of intermolecular interactions, which are relevant to the design of nanocomposites and to the calculations of phase equilibria and separation processes. He has built new QSPR multivariate nonlinear models based on artificial neural network and DFT for the estimation of the physical-chemical properties of compounds using COSMO sigma moments as molecular descriptors. His vapor-liquid equilibrium and evaporation models are based on the combination of the COSMO-RS theory and the CFD methodology.

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