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Quasielastic neutron scattering study of the dynamics of 1,3-diphenylpropane grafted to the pore surface of MCM-41 EDWARD KINTZEL, KENNETH HERWIG, MICHELLE KIDDER, A.C. BUCHANAN, PHILLIP BRITT, Oak Ridge National Laboratory, ALAN CHAFFE, Monash University — An initial study of the dynamics of 1,3-diphenylpropane (DPP, ≡Si-O-$C_6H_4(CH_2)_3C_6H_5$) attached to the surface of the mesoporous silica MCM-41 has been carried out using quasielastic neutron scattering. Measurements of the elastic intensity were carried out in the temperature range 50-380 K and indicate a trend in DPP dynamics with changing grafting density and pore size. Full quasielastic scans over an energy range of ± 17 μeV were carried out at temperatures of 240 K, 280 K, and 320 K. Initial analysis employed a stretched exponential to model the Fourier transformed data in the time domain. An average relaxation time, defined as $< \tau > = (\tau/\beta)\Gamma(1/\beta)$ where β is the stretched exponent in the model, shows a dependence on temperature, pore size, and DPP grafting density. Molecular dynamics simulations using a model for DPP grafted onto the surface of MCM-41 was compared with the experimental results.

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