

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Adsorption and Transport of Methane Molecules through One-Dimensional Channels in Dipeptide-Based Materials DANIELE PARADISO, Department of Chemistry, University of Tennessee, Knoxville, TN, United States, ENRICO PERELLI CIPPO, CNR - IFP, Milano, Italy, GIUSEPPE GORINI, Department of Physics, Milano-Bicocca University, Milano, Italy, GIORGIO ROSSI, Department of Physics, Università degli Studi di Milano, Milano, Italy, JOHN Z. LARESE, Department of Chemistry, University of Tennessee, Knoxville, TN, United States — The development of new materials for use in energy and environmental applications is of great interest, in particular in the areas of gas separation and carbon capture, where molecular transport plays a significant role. The dipeptides are organic molecules that offer an attractive possibility in such areas, because they form open hexagonal crystalline structures (space group P61) with quasi one-dimensional channels of tunable pore diameters in the range 3-6 Å. These molecular crystals exhibit selective adsorption, as well as, water and gas transport properties: these are believed to result from collective vibrations of the crystal structure that are coupled to the motions of the guest molecules within the channels. Current studies focus on characterizing the system methane and L-Isoleucyl-L-Valine (IV): this was initially done with high-resolution adsorption isotherms; then, high-resolution Inelastic Neutron Scattering measurements at the Spallation Neutron Source (BASIS spectrometer) revealed clear rotational tunneling peaks, offering details to unravel the potential energy surface of the system, as well as, evidences that channels flexibility and dynamical motion of the molecules have influence on the dipeptides adsorption properties.

Daniele Paradiso
University of Tennessee

Date submitted: 08 Jan 2016

Electronic form version 1.4