Stimuli Thresholds for Isomerization-Induced Molecular Motions in Azobenzene-Containing Materials.

Titre	Stimuli Thresholds for Isomerization-Induced Molecular Motions in Azobenzene-Containing Materials.
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Résumé en anglais	We use large-scale molecular dynamics simulations of the isomerizations of azobenzene molecules diluted inside a simple molecular material to investigate the effect of a modification of the cis isomer shape on the induced diffusion mechanism. To this end we simulate incomplete isomerizations, modifying the amplitude of the trans-to-cis isomerization. We find thresholds in the evolution of the host molecules mobility with the isomerization amplitude, a result predicted by the cage-breaking mechanism hypothesis (Teboul, V.; Saiddine, M.; Nunzi, J. M.; Accary, J. B. J. Chem. Phys. 2011, 134, 114517) and by the gradient pressure mechanism theory (Barrett, C. J.; Rochon, P. L.; Natansohn, A. L. J. Chem. Phys. 1998, 109, 1505–1516.). Above the threshold the diffusion then increases linearly with the variation of the chromophore size induced by the isomerization.
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[1] http://okina.univ-angers.fr/v.teboul/publications
[2] http://okina.univ-angers.fr/publications/ua8594
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