J Material Sci Eng 2015, 4:3
http://dx.doi.org/10.4172/2169-0022.S1.020

Click Chemistry; A Facile Route for Shape Memory Polymers

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Shape memory polymers (SMPs)are capable of holding a metastable shape (energy storage) and can deliver macro-scale shape (energy release) uponselective stimulus such as heat, current, magnetic field, pHand so on. Of various chemistries emerged, click chemistry, especially, copper catalyzed azide-lakynecycloaddition (CuAAC) reactions are being evolved recently to generate variety of SMPs. SMPs with trigger temperature above and below 100 °C (classified as high and low trigger temperature SMPs) can be synthesizedby this route in a very convenient way. The triazole links are very flexible which provide good shape recovery features for these SMPs. Dual trigger temperature SMPs are also synthesized by altering the composition of propargyl monomers in $A_3B_2B_3$ class polymers. Dual stimulus SMPs are another branch of SMPs, they can be stimulated by heat as well as by solvents at body temperature. The strikingfeature is that, the same cross-linked polytriazole can be used for aerospace application as well as for biomedical applications. High recovery stress SMPs have a special distinction which can also be realized by preparing elastic memory composites based on polytriazoles.

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Theoretical simulations of infrared spectra and multidimensional proton tunneling in hydrogen-bonded materials

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Theoretical model is presented for the X-H(D) stretching vibrations in hydrogen-bonded systems. The model takes into account an adiabatic coupling between the high-frequency X-H(D) stretching and the low-frequency intermolecular X...Y stretching modes, linear and quadratic distortions of the potential energy for the low-frequency vibrations in the excited state of the X-H(D) stretching vibration, resonance interactions between hydrogen bonds, and Fermi resonance between the X-H(D) stretching and the overtone of the X-H(D) bending vibrations. The effects of deuteration and temperature on spectra are successfully reproduced by the model. Comparison between experimental and theoretical spectra is presented for hydrogen- bonded crystals, liquids, gaseous complexes, as well as for ices and aqueous ionic solutions. Multidimensional proton tunneling in symmetric hydrogen-bonded systems is described by two-dimensional model potentials. The potentials have been fitted to quantum-mechanically calculated two-dimensional grid of energies, and used to analyze proton dynamics in tropolone. The model PES quantitatively reproduces experimentally observed promotion of the tunneling by the excitation of the planar modes and suppression by the excitation of the out-of-plane modes.

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