Poster Presentation

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Design of Mechanically Flexible Organic Crystals: A Crystal Engineering Approach

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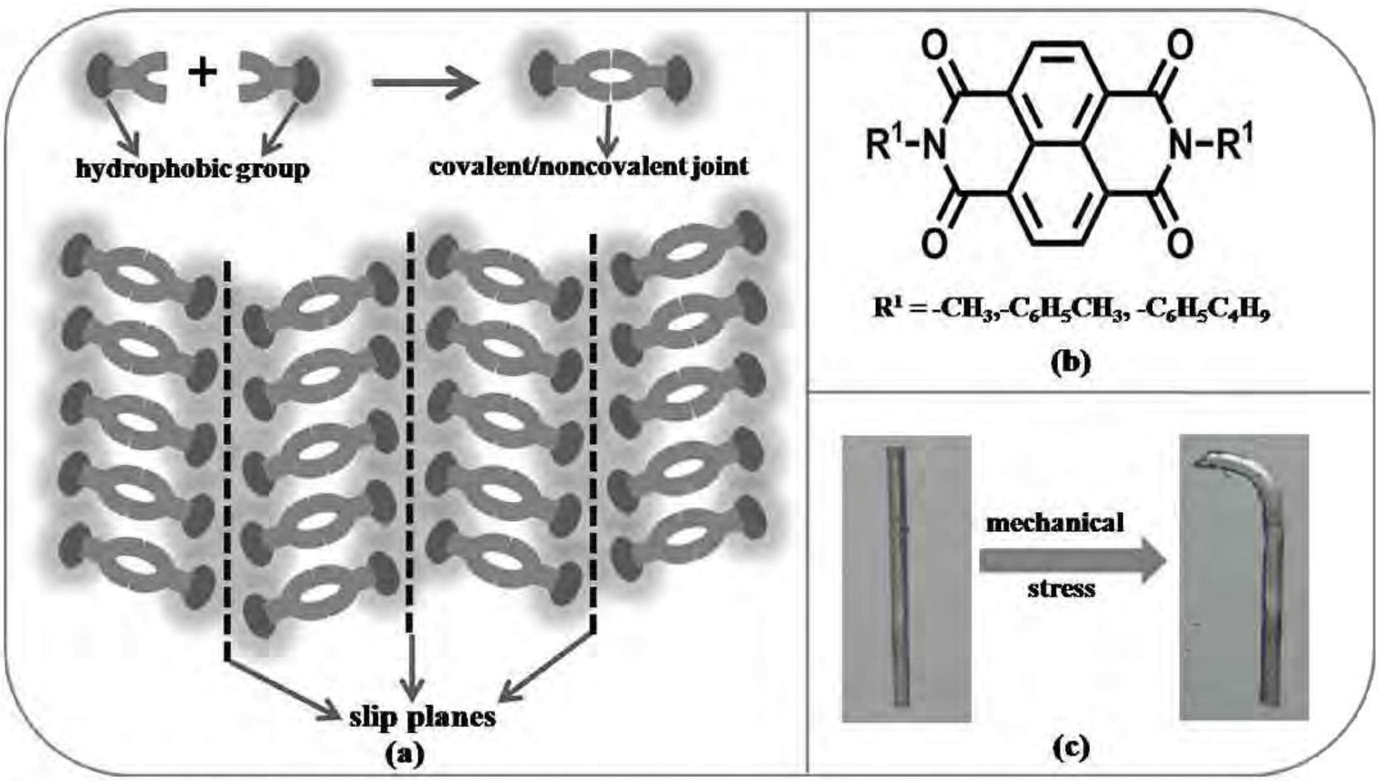
Utilization of organic single crystal materials is increasing day by day owing to their promising applications in organic light emitting diodes [1], organic solar cells, mechanochromic luminescence [2] and tablatability [3] of APIs etc. These desirable functions, especially mechanical properties, can be achieved by imparting soft nature in organic materials, however unfortunately there is no simple strategy to attain this. Till date all the findings are serendipitous discoveries, so a rational design strategy is necessary to accomplish such soft mechanical behavior in molecular crystals. Here we propose a design strategy to attain plastically deformable organic materials by introducing slip planes in the crystal structures. The high plasticity can be achieved by introducing hydrophobic groups, such as t-Bu, -OMe, -Me and multiple –Cl (or) –Br groups on -Ar building blocks, for example on naphthalene diimide (NDI), which leads to the formation of slip planes in the crystal structures (as shown in attached figure), hence facilitate the plastic (irreversible) bending [2].

[1] *A. L. Briseno et al. Nature., 2006, 444, 913-917,* ***[2]*** *G. R. Krishna et al. Adv. Funct. Mater., 2013, 23, 1422-1430,* ***[3]*** *P. P. Bag et al. Cryst EngComm., 2012, 14, 3865-3867*



Scheme 1: (a) A schematic representation of the target crystal packing. (b) Chemical structures of NDI derivatives. (c) Crystal undergoing bending deformation on application of a mechanical stress.

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