STRAIN ENGINEERING TO UNDERSTAND AND AMPLIFY ANOMALOUS BEHAVIOUR IN FRAMEWORK MATERIALS FOR ENERGY APPLICATIONS

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The designable architecture of framework materials endows many with a macroscopic behaviour seldom found in more traditional solid-state materials [1]. While this anomalous behaviour is interesting for novel applications, it remains challenging to identify (i) which materials show potential for such behaviour and (ii) how to amplify this behaviour. We recently developed strain engineering as an *in silico* approach to answer these questions [2]. Herein, we will illustrate strain engineering *via* two case studies and illustrate the open challenges to develop it into a widely applicable design tool. We first focus on the UiO-66 metal-organic framework (MOF). By creating well-defined linker vacancies, this rigid material becomes locally flexible [2]. The so-created reversible crumple zones also focus the strain, thereby preserving the integrity and adsorption capacity of the remainder of the material (Fig. 1), which may find applications in shock absorbers. The second case study explores how to induce stimuli-induced phase coexistence in the soft porous crystals CoBDP, DMOF-1(Zn), and MIL-53(Al)-F [2,3]. We demonstrate that increasing the temperature or adsorbing guests leads to a dynamic redistribution of the strain disfavouring phase coexistence, which can in turn be exploited to control these materials' polymorphism [2].

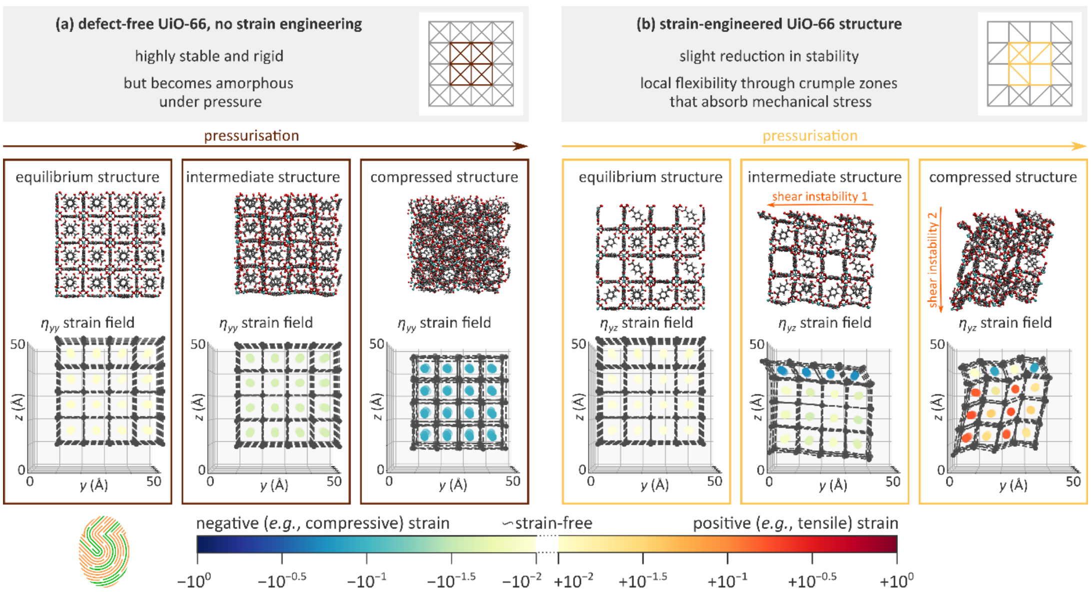

Figure 1: Introducing flexibility into the rigid UiO-66 MOF through strain engineering [2].

References

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