MS29-1-7 The Elastic Properties of Postulated Solid Forms from First Principles
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R. Zwane [1]
[1]**Dublin City University - Dublin (Ireland)**

Abstract
The elastic properties of a crystal contain extensive information about the response of a material to applied stress and strain and influence key properties such as hardness, powder flexibility, and tabletability. Different polymorphs and solid forms of an active pharmaceutical ingredient (API) can exhibit markedly different elastic and mechanical properties, and therefore understanding the mechanical properties of different solid forms would greatly aid pharmaceutical solid-form development. In crystal structure predictiion, the analysis of a crystal energy landscape in a pharmaceutical setting can aid the understanding of polymorphism of an API across a landscape and assist in identifying mechanical properties accessible to an API. In this contribution, mechanical properties of postulated solid forms of 2-((4-(3,4-Dichlorophenethyl)phenyl)amino)benzoic acid DPAB, utilized for the treatment of Alzheimer's disease and the XXIIIth molecule in the sixth CSP blind test, are characterized using first-principles and first-principles based methods (density-functional theory). The assessment of mechanical stability, elastic moduli and the anisotropy of the elastic moduli of DPAB will potentially enable the screening of putative solid forms for a polymorph(s) that exhibits improved compression properties.
image caption

References
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