The Flexibility Window

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Functionally interesting materials often exist in the flexibility window which lies between rigid materials (e.g. crystalline silicon) that cannot deform and flexible materials that can adopt multiple distinct conformations (e.g. polymer chains). The nature of the interatomic interactions makes some materials rigid while others are flexible. This is controlled by constraints, both equalities and inequalities, which determine the flexible and rigid regions. Graph theory methods are used to find the flexibility and geometric simulation methods are used to study the mobility.

Examples include (a) zeolites maximize their density and contain flexible pores that are useful for cracking petroleum (b) the intermediate phase in chalcogenide glasses that has unusual reversibility properties and (c) proteins and other biomolecules that have enough rigidity to define their three dimensional structure, while retaining enough flexibility to function (d) quadrupolar ordering of the corner sharing octahedra in $LaMnO_3$.

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