

Architecture and Co-Evolution of Allosteric Materials

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We introduce a numerical scheme to evolve functional materials that can accomplish a specified mechanical task. In this scheme, the number of solutions, their spatial architectures and the correlations among them can be computed. As an example, we consider an "allosteric" task, which requires the material to respond specifically to a stimulus at a distant active site. We find that functioning materials evolve a less-constrained trumpet-shaped region connecting the stimulus and active sites and that the amplitude of the elastic response varies non-monotonically along the trumpet. As previously shown for some proteins, we find that correlations appearing during evolution alone are sufficient to identify key aspects of this design. Finally, we show that the success of this architecture stems from the emergence of soft edge modes recently found to appear near the surface of marginally connected materials. Overall, our *in silico* evolution experiment offers a new window to study the relationship between structure, function, and correlations emerging during evolution.

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