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Architecture of Allosteric Materials and Edge Modes[1] LE YAN, Kavli Institute for Theoretical Physics, UCSB, RICCARDO RAVASIO, Institute of Physics, EPFL, CAROLINA BRITO, Instituto de Fisica, Universidade Federal do Rio Grande, MATTHIEU WYART, Institute of Physics, EPFL — Allostery, a long-range elasticity-mediated interaction, remains the biggest mystery decades after its discovery in proteins. 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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