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Stiffness of Diphenylalanine-Based Molecular Solids from First Principles Calculations IDO AZURI, Weizmann Institute of Science, Israel, ODED HOD, EHUD GAZIT, Tel Aviv University, Israel, LEEOR KRONIK, Weizmann Institute of Science, Israel — Diphenylalanine-based peptide nanotubes were found to be unexpectedly stiff, with a Young modulus of 19 GPa. Here, we calculate the Young modulus from first principles, using density functional theory with dispersive corrections. This allows us to show that at least half of the stiffness of the material comes from dispersive interactions and to identify the nature of the interactions that contribute most to the stiffness. This presents a general strategy for the analysis of bioinspired functional materials.

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