From prediction of structure to design of function

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I will first describe recent progress in high resolution macromolecular structure prediction, and show that models with atomic level accuracy can now be routinely generated using Rosetta with the incorporation of even limited experimental data to guide the conformational search. I will then describe the computer based design of proteins with novel functions, in particular enzyme catalysts for reactions not catalyzed by naturally occurring enzymes. I will close by describing our efforts to channel the energy and brainpower of lay people around the world into protein science through foldit, a multiplayer online computer game.