Designing biomimetic materials that exhibit adaptive functionality and are capable of retaining this functionality in harsh environments is vital for a range of applications. I will introduce a few examples of how computational modeling can be used to facilitate design of such biomimetic systems. In the first part of my talk, I will focus on active magnetoelastic gel-based composites. In the second part of my talk, I will focus on the design of highly thermostable copolymer-enzyme complexes. Enzymes are environmentally friendly and safe catalysts that accelerate a range of chemical reactions by many orders of magnitude. I will show that by conjugating lysozymes with copolymers with tailored architectures it is possible to dramatically improve their thermal stability well beyond that of native enzymes. This strategy could be suitable for a variety of applications incorporating enzymes into engineering materials and thereby could find its use in a range of applications, from the deactivation of toxic materials and biomedical applications to biological fuel cells.