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The molecular electronics of protein fragments¹ DAVID CARDA-MONE, GEORGE KIRCZENOW, Simon Fraser University — Small fragments of polypeptide chains provide a uniquely scalable, customizable basis for nanoelectronic devices. Using a combination of *ab initio* and semi-empirical techniques, we arrive at a quantitative understanding of the charge transport properties of these molecules. This allows us to investigate their chemical and physical properties, such as lead-molecule bonding geometry, lead-induced distortion of molecular structure (e.g., molecular stretching), and device properties. We explain the observed current rectification in these molecules and further predict negative differential resistance, opening the way to protein-based nanoelectronic devices.

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