There have been many studies of experiments with hydrogen or deuterium in metals reporting anomalous reactions, described as LENR or CANR or cold fusion. Understanding and optimization of the effect would be helped if testable hypotheses could be found that can account for the many remarkable anomalies. Here chemical conditions associated with the anomalies are modeled using standard ab initio computational chemistry software, so validity of the calculation method is transparent and replicable. Here models of LENR chemical environments suggest ways the anomalies can be triggered, optimized, and tested.