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Aspects of selenium redox (bio)chemistry disclosed *in silico*

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Exactly 50 years ago, selenium was linked to glutathione peroxidase: the beginning of selenium enzymology was marked, thus initiating the still running debate on the role of this oligoelement in biology. Focusing on the capacity of Se-containing molecules and biomolecules to reduce hydroperoxides, we have explored *in silico* the elementary steps in which selenium presence is crucial. Through selected examples from chemistry and biology, by using results from accurate quantum mechanical modelling, we provide a unified picture of selenium's unique capacity of reducing hydroperoxides. Common to all these systems is the nucleophilic attack of selenium to one oxygen of the peroxide bond promoting its disruption. The redox properties of selenium, compared to those of its siblings sulfur and tellurium, makes this chalcogen a unique reactive center. Spanning the range of the biologically relevant chalcogen oxidation numbers, the observed peculiar reactivity of selenium can be explained also in other reactions, for example in chalcogenoxides eliminations, which, despite their synthetic utility to introduce a carbon-carbon double bond in an organic scaffold, lead to deselenylation and thus irreversible enzyme inactivation in the biological environment.