Quantum chemical methods help unravel effects of pH on marine communication

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Marine organisms use a large variety of small chemical compounds to communicate. These signalling molecules are used, for example, to detect predators, find mating partners, locate the best place to settle or the next meal. Increasing amounts of atmospheric CO_2 that dissolve into the oceans cause a drop of ocean pH. This process called ocean acidification is known to affect the physiology and fitness of organisms. Lately it has also been reported to affect numerous animal behaviours that are mediated by chemical signalling cues. However, little is known about the underlying mechanisms, especially in invertebrates.

We investigate the molecular effects of decreasing ocean pH on the structure and function of peptide signalling cues as one potential mechanism to explain altered animal behaviour in high CO_2 conditions. This requires a multi-disciplinary approach including NMR spectroscopy to determine the peptide cues' susceptibility to protonation and quantum chemical calculations to explore the differences in conformation and charge distribution of the relevant protonation states. Here we present first results of our structural molecular investigation and highlight the quantum chemical methods required to successfully model molecular conformation and molecular electrostatic potential in solution.