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Anionic States play more important role: Electronic Structure Informatics of Gas-Phase Acidity Toward Fast and Precise Acids Design for Engineering

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Abstract (less than 300 words)

In semiconductor processing, it is necessary to design super acids having desired physicochemical properties according to the situation where they will be applied. In acid engineering, there is a growing momentum breaking away from the traditional experiment-driven molecular design in which whole candidates are synthesized. Since the synthesis of superacid is dangerous, it has been considered necessary to design the target superacid molecule safely with enough quickness and precision before experiments. For this purpose, there is a need to develop a new theoretical molecular design method based on quantum chemical calculations that can predict the acidity of unknown compounds. Acid pK_a values can be calculated by quantum chemical methods with an error of about 1 pK_a from the experimental value. However, previous methods require manual classification of the acidity functional group for each compound species [1], and there is no highly accurate and efficient method for predicting the acidity of arbitrary compounds.

We have performed a set of *ab initio* molecular orbital calculations to predict the gas phase acidities of various organic substances, which is the basis of superacid design. We confirmed the necessity of high-precision quantum chemical calculations that can accurately calculate the anions. In general, the high-precision molecular orbital method has been considered unsuitable for the industrial exploration of new super-acidic materials due to its high computational cost. In this study, we report on developing a method for fast prediction of gas-phase acidity (calculation time/molecule: 1 day → 1 min) using machine learning models with the results of the high-precision molecular orbital method as the correct answer information. This method quantitatively suggests that it is necessary to consider the anionic state to explain acidity and that accurate prediction cannot be expected from the neutral state only.

References

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