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Identification of Defects in Materials: A Combination of First-principles Calculations and Experiments

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It is well known that many physical properties of materials can be determined by the existence of point defects, which might be intentionally or accidentally added to the materials. For example, the electrical conductivity of Al-doped ZnO sample can be decreased by the presence of Zn vacancy (V_{Zn}) defect, which might be unintentionally created under O-rich growth conditions. In addition, the hydrogen defect is also reported to be a major obstacle for achieving p-type ZnO. Therefore, understanding the role of defects in materials can help us improving the material properties in a desired way. By combining the first-principles calculations with proper characterization techniques, such as x-ray absorption, infrared absorption, and photoluminescence, defects in materials can be understood in a great detail. A few examples, including Al-doped ZnO, SO-doped CdTe and N-doped Cu₂O, will be presented.

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