

**O35 | Combining experiments and theory in positron annihilation techniques:  
recent advances and future prospects**

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The collaboration between positron annihilation experiments and supporting theoretical modeling has been especially fruitful in the identification of vacancy defects in crystalline matter [1] such as semiconductors, metals and alloys. As the structural complexity of the materials systems studied continues to increase, a larger number of defect candidates have to be considered computationally in order to be able to understand trends seen in experiments and the defects or defect complexes are behind the measured data. This is usually the case in positron studies of complex oxides [2] where cation vacancies are usually complexed with one or more oxygen vacancies, in semiconductor alloys [3] or in multicomponent metallic alloys [4], in which point defects occur in many different atomic configurations. In best cases, thorough experimental work combined with simulations can provide a very detailed picture of the structural and chemical identities of vacancy defects detected [5].

The two-component density functional theory, which is typically the preferred method in defect studies, can quite reliably predict the ground-state of a thermalized positron in a given defect or nanostructure model in solid-state matter. On the other hand, correlated positron states such as surface states are difficult or even impossible to model using existing correlation functionals. In addition to the electron-positron correlation energy and potential, especially the positron annihilation rate and momentum density of annihilation radiation, are difficult to describe in a density-functional formalism.

In this talk, I will discuss some of our past works combining experiment and theory in defect identification. The examples include semiconductors, complex oxides and metallic alloys. I will also discuss some future prospects and ongoing methodological developments. For example, how recent advances of electronic-structure methods could, in principle, be adapted to calculating defect and charge-state-specific trapping rates in semiconductors. Most importantly, I will discuss our preliminary work beyond density-functional theory, namely applying quantum Monte Carlo methods to positrons in condensed matter systems [6].

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