Studying ZnO/ZnS heterostructures by solid-state NMR (reveals mechanistic aspects of ZnO sulfidation process)

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Semiconducting heterostructures are considered potential options for applications such as energy production, pollution control, and sensing. Optimizing the performance of these systems depends on a thorough understanding of their formation mechanisms in relation to their synthesis methods.

This study focused on ZnO/ZnS heterostructures composed of a ZnO core and ZnS shell. These nanoscale heterostructures, with different O/S stoichiometries, were produced from ZnO nanoparticles through a sulfidation reaction using anion exchange under mild conditions.

Multinuclear ^{13}C CP-MAS NMR experiments were performed on ZnO/ZnS materials to monitor their surface state by examining the preferred conformation of surfactants on the ZnO and ZnS regions. The presence of the ZnO phase allowed analysis of the local environment of O-atoms using ^{17}O NMR. Selective labeling with ^{17}O-water and extensive quantitative data on sulfidation kinetics enabled distinction between surface and core O-atoms. In particular, O-atoms at the ZnO/ZnS interfaces were characterized and quantified based on the degree of sulfidation.

The results demonstrate a methodological NMR approach applicable to other materials for relating macroscopic properties to atomic structure.