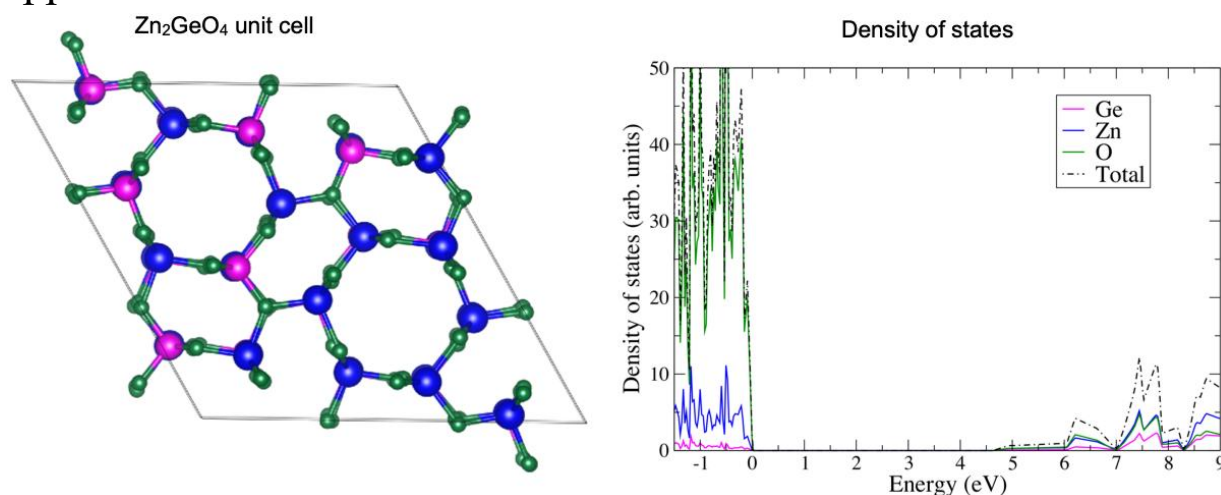


Prof. Ruth Martínez Casado

Complutense University of Madrid (Spain)

Density functional theory (DFT): calculations and experimental validation

Density Functional Theory (DFT) is one of the most widely used computational methods to investigate the electronic structure of materials. In this talk, an intuitive overview of DFT will be presented, with emphasis on its practical applications in materials science. Examples will illustrate how DFT can be used to predict structural, electronic, and magnetic properties, as well as its role in the design of functional materials. The main limitations of the method, including the band gap problem, will also be briefly discussed. This lecture aims to highlight DFT as a powerful tool connecting quantum mechanics with real-world applications.



Donnerstag, 23.04.2026 um 17:15 Uhr in Hörsaal B



**Westfälische
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