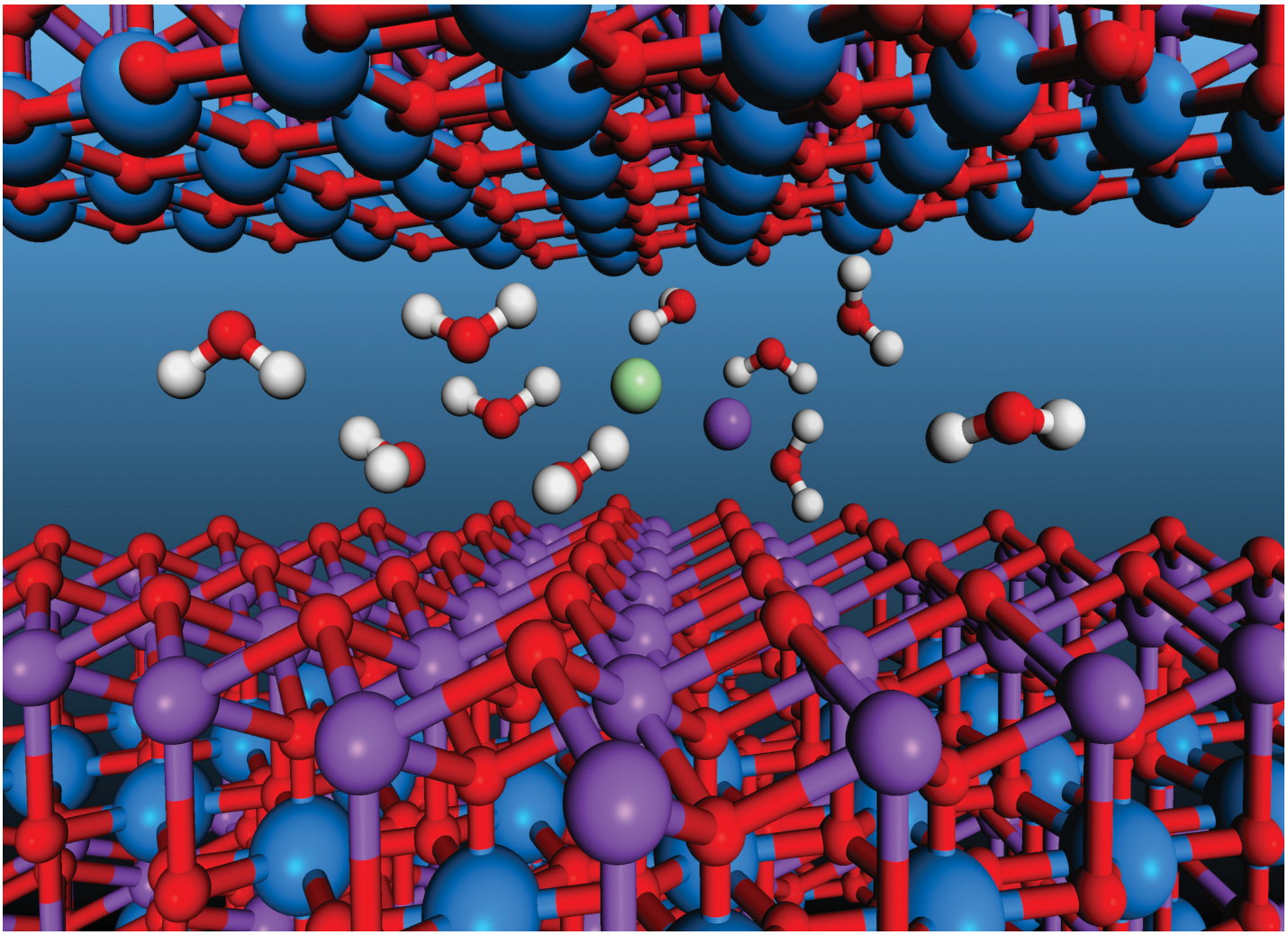

Showcasing computational research from Dr Philippe F. Weck and Dr Carlos F. Jové-Colón at Sandia National Laboratories and from Prof. Eunja Kim at The University of Texas at El Paso.

Polymorphism and phase transitions in $Na_2U_2O_7$ from density functional perturbation theory

Polymorphism and phase transitions in sodium diuranate, $Na_2U_2O_7$, are investigated with density functional perturbation theory. Thermal properties of crystalline α-, β- and γ-$Na_2U_2O_7$ polymorphs are predicted from phonon calculations, *i.e.*, the first time for the high-temperature γ-$Na_2U_2O_7$ phase. Gibbs free energy calculations do no predict a direct $\beta \rightarrow \gamma$ solid–solid phase transition, but suggest instead the occurrence of a multi-step process consisting of initial β-phase decomposition, followed by recrystallization into γ-phase at high temperature.

As featured in:

See Philippe F. Weck *et al.*, *Phys. Chem. Chem. Phys.*, 2023, **25**, 16727.

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