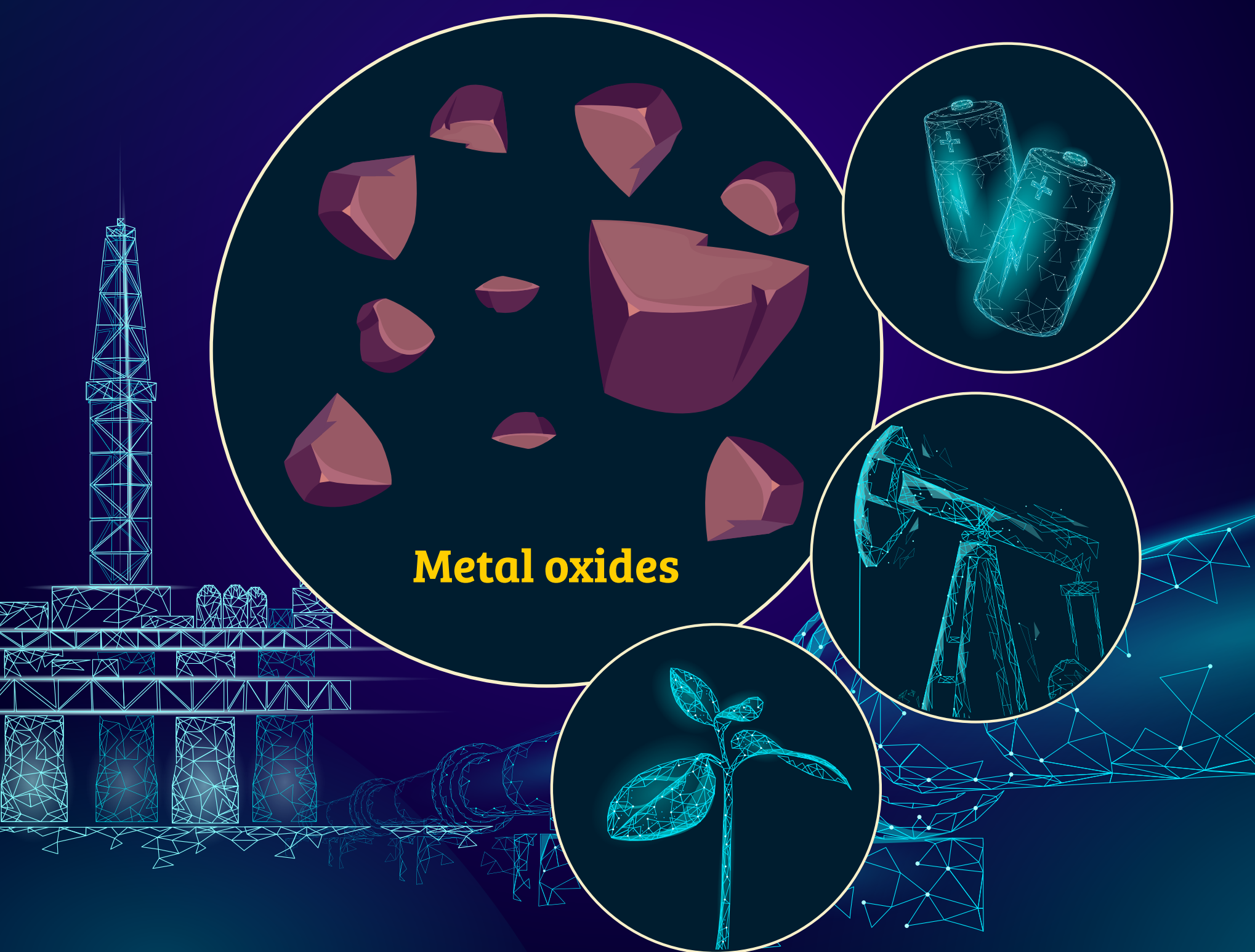


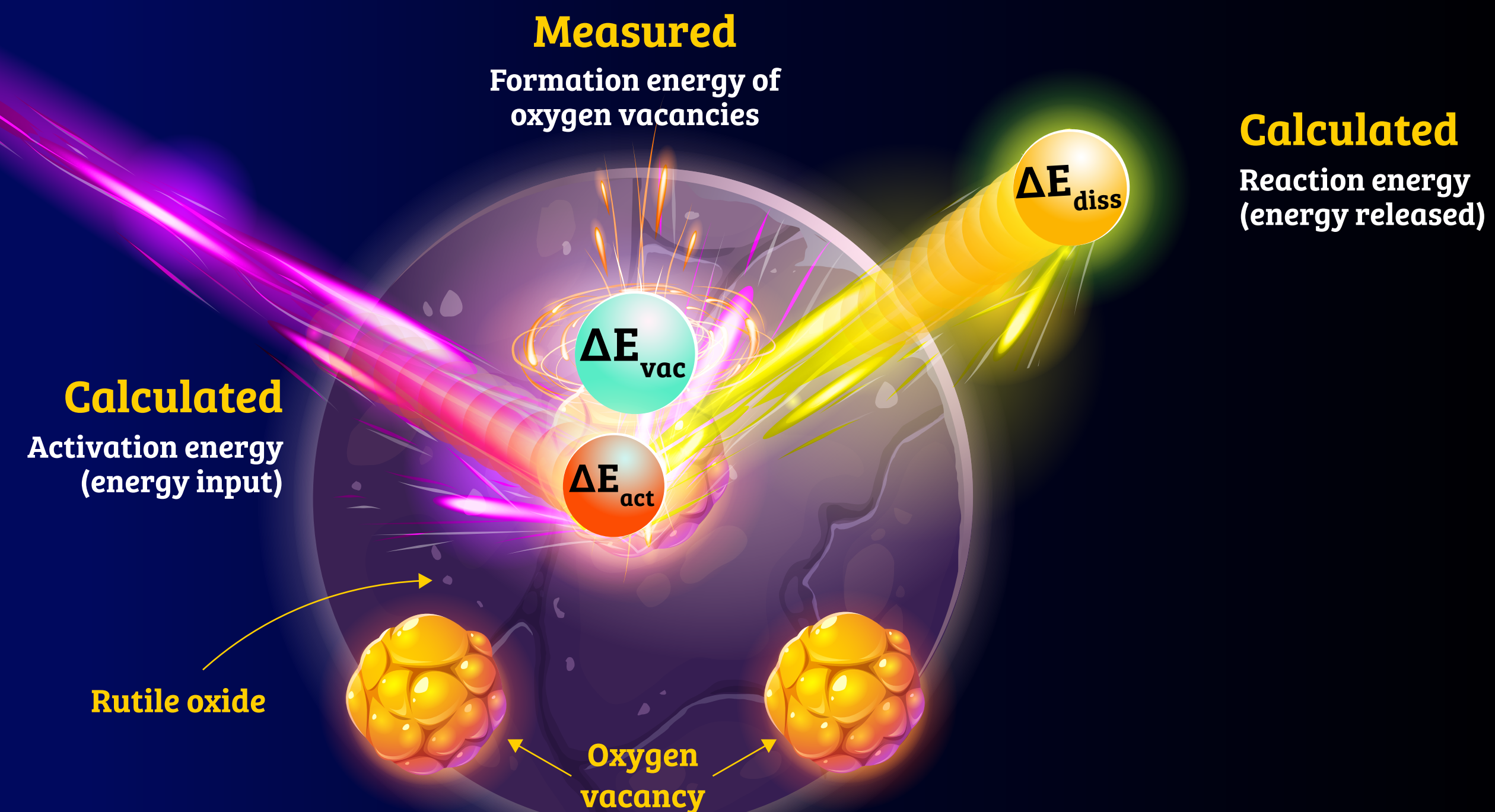
Oxygen Vacancies: An Easier Road to Predicting Metal Oxide Catalysis

Metal oxide catalysts have numerous industrial applications, so it is important to understand the dynamics of their catalytic activities



However, the energy input required for catalysis on their surfaces is tedious to calculate

Can the energy input be estimated using a simpler property of metal oxides?



ΔE_{vac} (measurable and easily computable) is a simple and accurate descriptor of ΔE_{act} and ΔE_{diss} (both tedious to calculate) for rutile oxides

By using ΔE_{vac} to determine the more complex ΔE_{act} , rutile oxide catalyst designs can be enhanced for their more efficient industrial application