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NEWS | FEBRUARY 10 2023

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Scilight 2023, 061107 (2023)
https://doi.org/10.1063/10.0017265

AIP Publishing

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10 February 2023

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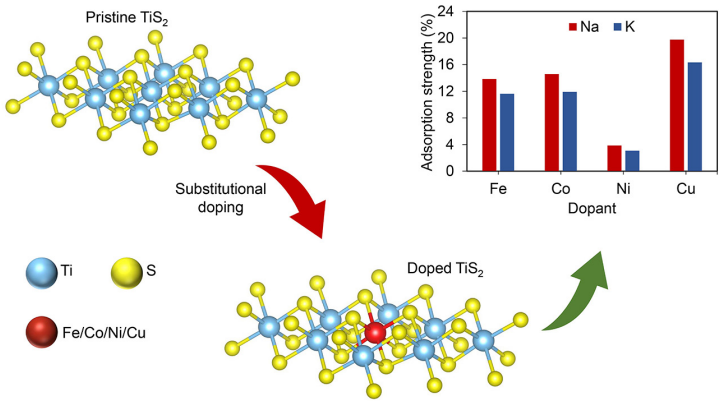
Density Functional Theory models point to potential for new anode material in next-generation batteries.



Most of today's electronics and electric vehicles rely on batteries in which relatively low-capacity graphite is used for anodes. Two-dimensional titanium disulfide (TiS_2) has shown promise as an alternative nanomaterial due to its superior absorption and diffusion of sodium and potassium ions and because it is among the lightest transition metal dichalcogenides.

Using first-principles Density Functional Theory (DFT), researchers investigated the adsorption and diffusion of sodium and potassium ions on doped TiS_2 monolayers. By applying DFT simulations in which titanium was substituted by other transition metals with 3d electron configurations, Nair et al. described how 2D TiS_2 not only outperforms graphite as a potential anode material but can be enhanced further by doping.

"We predicted significant improvements in the adsorption energies of sodium and potassium ions in all doped cases, of up to 20% for copper-doped TiS_2," said author Akhil Nair. "Additionally, the average open circuit voltage rose considerably, by more than 60%, when sodium ions were absorbed by TiS_2 monolayers doped with iron or cobalt."

The group hopes to continue investigating the potential for 2D materials in batteries and to develop a modeling-experimental framework for battery material discovery.

"Our results suggest that 2D TiS_2 has remarkable adsorption and diffusion properties that could be significantly enhanced by transition-metal doping, making it an attractive material for alkali-ion battery anodes," said author Carlos Da Silva. "We believe this publication will encourage researchers to further investigate the tuning strategy used in our study to optimize the properties of different nanomaterials for battery anodes."

Source: "Dopant-enhanced sodium and potassium-ion adsorption and diffusion in two-dimensional titanium disulfide," by A. K. Nair, C. M. Da Silva, and C. H. Amon, *Journal of Applied Physics* (2023). The article can be accessed at https://doi.org/10.1063/5.0132894.