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**Capping Repels Oxygen and Selectively Adsorbs Hydrogen via Kubas Interaction** RAFIA AHMAD, ABHISHEK K. SINGH, Materials Research Centre, Indian Institute of Science Bangalore — Hydrogen bound via Kubas interaction on metal decorated light weight materials forebodes a much efficient alternative for the fast depleting fossil fuels. $O_2$ interference in hydrogen storage on metal decorated carbonaceous systems remains one of the major stumbling blocks in successful realization of the theoretically promised high storage of Kubas bound $H_2$. The interference is a consequence of preferred $O_2$ binding at the metal site, thereby blocking it for $H_2$ adsorption. Here, we report that arene capping of a Sc-metallacarborane (MCB) efficiently reverses the preferential adsorption of $O_2$ over $H_2$. The capped Sc-MCB completely repels $O_2$ off the Sc-site allowing solely Kubas binding of $H_2$, consequent of the down-shift of the $d$-band center of Sc from 1.29 eV in the uncapped to 5.67 eV in the capped MCB, below the Fermi-level, respectively. This optimised $d$-band center position enables the empty Sc antibonding states to only be available for hydrogen adsorption via Kubas interaction, thereby, to completely avoid oxygen binding. This result provides an approach by tuning a cluster electronically to enhance gas adsorption selectivity, which can be efficiently ulitized in various catalytic, sensing and gas storage systems.

Rafia Ahmad
Indian Inst of Science

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