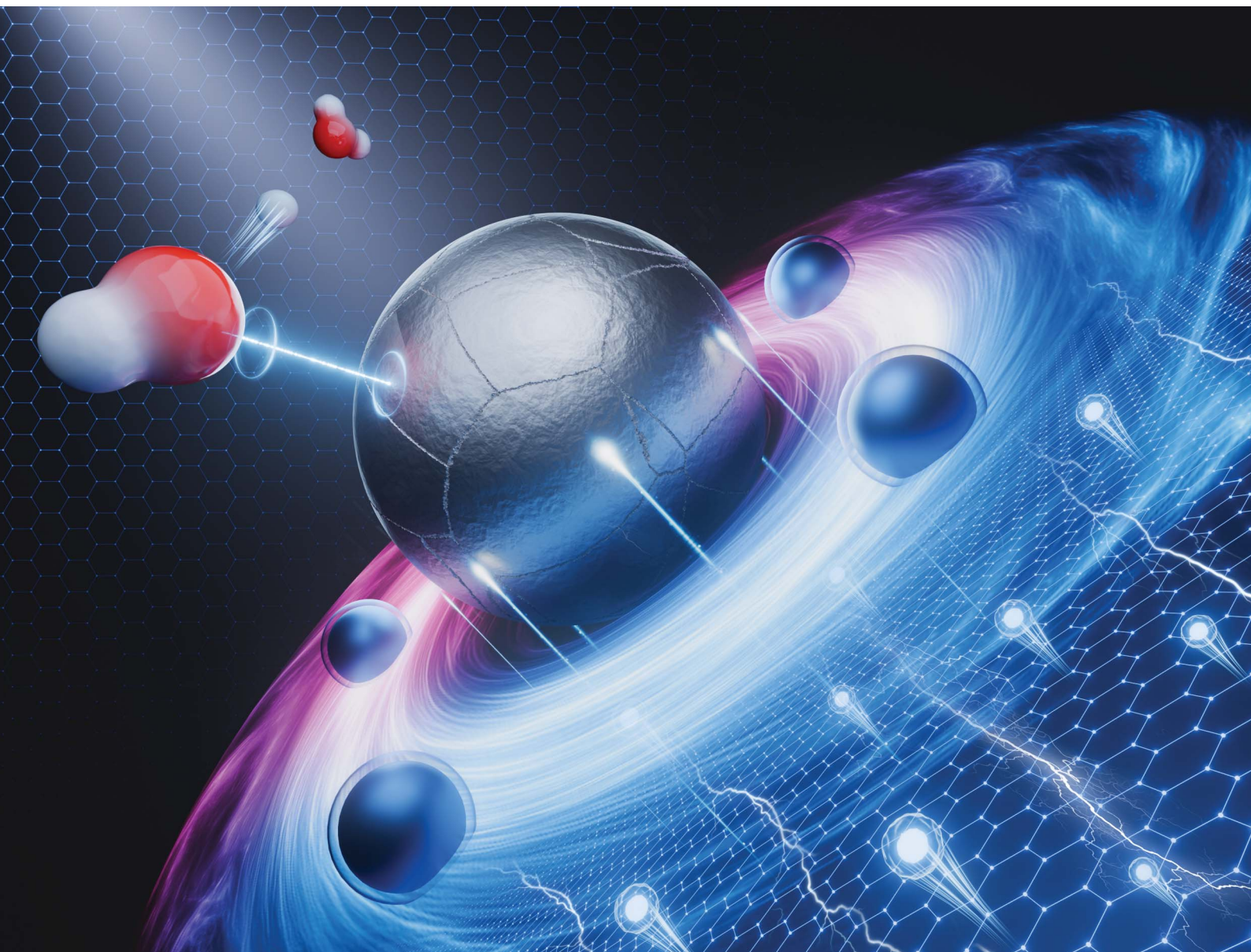


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Fubo Tian, Zhiyao Duan *et al.*

Deciphering potential-driven dynamics in Fe–N–C catalysts: *ab initio* insights into Fe–N switching and spin-state transition