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Two-dimensional materials for cost effective catalysts[1]

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Two dimensional (2D) materials are emerging with far-reaching potential for technical and industrial applications. Thanks to recent developments and improvement of production technologies, functionalization and scalable production of these cost-effective materials is becoming a reality, paving the way for their high volume applications. In this talk, after a brief review of current opportunities and challenges, I will discuss efforts at manipulating the chemical properties of two such materials for catalytic applications: single-layer molybdenum disulfide (MoS_2) and hexagonal boron nitride (h-BN). I will show that the basal plane of single-layer MoS_2, which is inherently inert, can serve as a ground for alcohol synthesis from syngas (combination of CO and H_2) in the presence of vacancies. Its reactivity and selectivity can be further optimized by tuning the location of frontier orbitals via the geometry of the vacancy clusters, and interface with a transition metal support. On the other hand, defect-laden basal plane of h-BN is found to be a metal-free catalyst for hydrogenation of olefins, which has great potential in variety of industrial applications.

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