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Catalytic effect of carbon nanomaterials on light metal hydride systems ZHAO QIAN, RAJEEV AHUJA, Cond. Mat. Theory Group, Dept of Physics and Astronomy, Uppsala Univ; Dept of Mat. Sci. and Eng., Royal Inst. of Tech. (KTH), Stockholm, Sweden, C. MOYSES ARAUJO, ANDREAS BLOMQVIST, BISWARUP PATHAK, RALPH H. SCHEICHER, CMT Group, Uppsala University — Carbon nanomaterials are becoming recognized for their use in catalyzing hydrogen desorption from light metal hydride systems, in particular complex borohydrides and alanates. For example, it was shown by us that graphene, carbon nanotubes, and especially fullerenes can improve the hydrogen sorption properties of sodium alanate [Nano Lett. 9, 1501 (2009)]. In parallel to ongoing experimental investigations, we have carried out further theoretical studies in order to better understand the underlying catalyzing mechanism. Our most recent work is concentrated on the interaction of lithium borohydride with fullerene where a complete dehydrogenation process was simulated using the cluster approach. Furthermore, the catalytic effect of graphene nanofibres on sodium alanate has been experimentally demonstrated by our collaborators, and we have studied this system from first principles as well, to better understand the origin of its catalytic effect.

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