Figures for supporting information.

Nanoscale curvature induced hydrogen adsorption in alkali metal doped carbon nanomaterials

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<u>Figure 1</u> Optimized structures of alkali metal atom doped C_{20} fullerenes (at 5m-ring) their hydrogen adsorption (at 5m-ring)

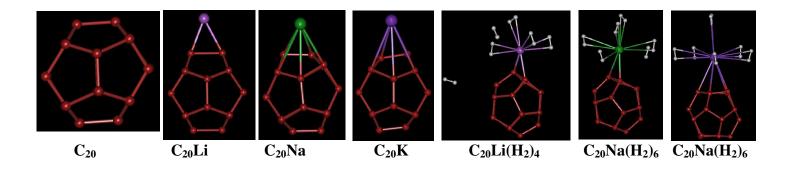
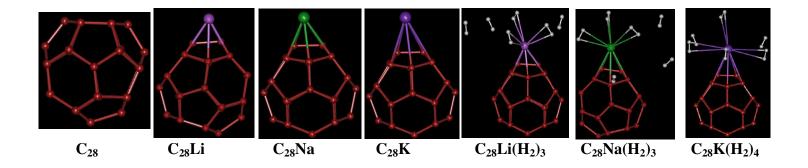
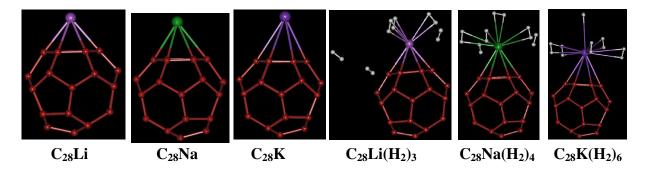


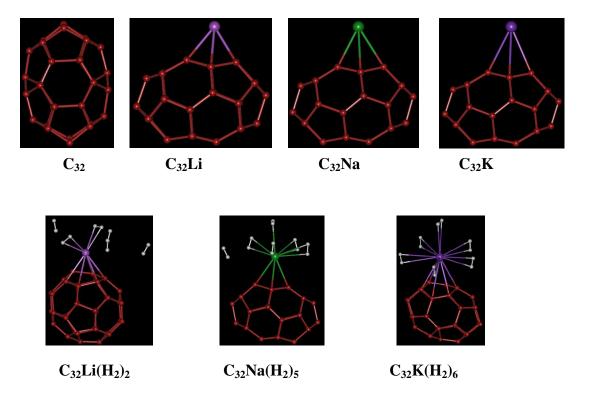
Figure 2a Optimized structures of alkali metal atom doped C_{28} and their hydrogen adsorption fullerenes (at 5m-ring



<u>Figure 2b</u> Optimized structures of alkali metal atom doped C_{28} fullerenes and their hydrogen adsorption (at 6m-ring)



<u>Figure 3a</u> Optimized structures of alkali metal atom doped C_{32} fullerenes and their hydrogen adsorption (at 6m-ring)

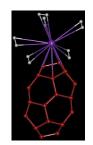


<u>Figure 3b</u> Optimized structures of alkali metal atom doped C_{32} fullerenes and their hydrogen adsorption (at 5m-ring)



 $C_{32}Li(H_2)_2 \\$

C₃₂Na(H₂)₆



 $C_{32}K(H_2)_6$

Figure 4a: Optimized structures of alkali metal atom doped C_{36} fullerenes and their hydrogen adsorption (at 5m-ring)

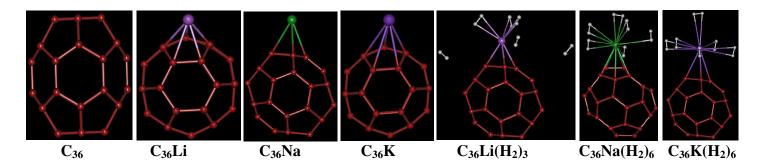


Figure 4b: Optimized structures of alkali metal atom doped C_{36} fullerenes and their hydrogen adsorption (at 6m-ring)

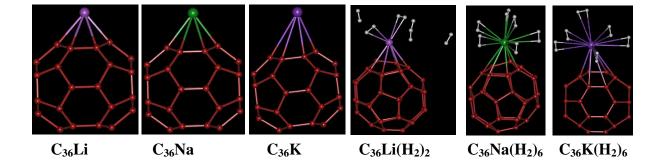
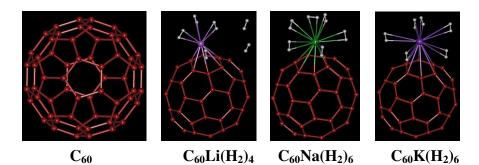
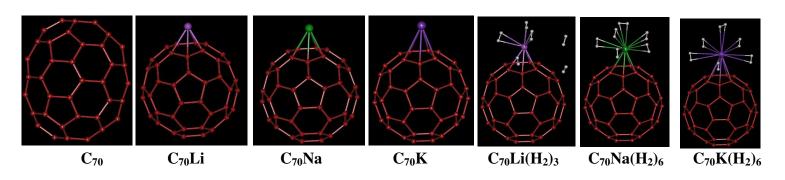


Figure 5a: Optimized structures of alkali metal atom doped C_{60} fullerene and their hydrogen adsorption (at 6m-ring)



<u>Figure 6a:</u> Optimized structures of alkali metal atom doped C₇₀ fullerenes and their hydrogen adsorption (at 5m-ring)



<u>Figure 6b:</u> Optimized structures of alkali metal atom doped C₇₀ fullerenes and their hydrogen adsorption (at 6m-ring)

