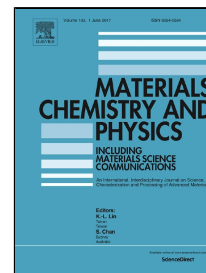


# Accepted Manuscript

Application of C<sub>60</sub>, C<sub>72</sub> and carbon nanotubes as anode for Lithium-ion batteries:  
A DFT study



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PII: S0254-0584(17)30315-2

DOI: 10.1016/j.matchemphys.2017.04.032

Reference: MAC 19634

To appear in: *Materials Chemistry and Physics*

Received Date: 09 December 2016

Revised Date: 04 April 2017

Accepted Date: 16 April 2017

Please cite this article as: Meysam Najafi, Application of C<sub>60</sub>, C<sub>72</sub> and carbon nanotubes as anode for Lithium-ion batteries: A DFT study, *Materials Chemistry and Physics* (2017), doi: 10.1016/j.matchemphys.2017.04.032

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## Highlighted

- $C_{60}$  and CNT (10, 0) as anode materials for Lithium-ion batteries were investigated
- $V_{\text{cell}}$  and  $E_{\text{ad}}$  of CNT (8, 0) and CNT (10, 0) were higher than  $C_{60}$  and  $C_{72}$  ca
- $\text{NH}_2$  functionalization of  $C_{60}$  improve the performance of it as anode materials of Lithium-ion batteries

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