

## Theoretical prediction of MoN<sub>2</sub> monolayer as a high capacity electrode material for metal ion batteries

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**Table SI** Electrochemical characteristics of current widely investigated cathode materials. And corresponding reference in article.

<sup>a</sup> Values without and within brackets are given for the theoretical and practical specific capacity of corresponding cathodes, respectively.

	Specific capacity <sup>a</sup> (mA h g <sup>-1</sup> )	Average potential (V vs. Li/Li <sup>+</sup> )	Reference
MoN <sub>2</sub> monolayer	432	3.64	Current work
LiCoO <sub>2</sub>	272 (140)	~4.2	<a href="#">54,55</a>
LiNi <sub>1/3</sub> Mn <sub>1/3</sub> Co <sub>1/3</sub> O <sub>2</sub>	272 (200)	~3.7	<a href="#">56</a>
LiMn <sub>2</sub> O <sub>4</sub>	148 (120)	~4.1	<a href="#">57</a>
LiFePO <sub>4</sub>	170 (160)	3.45	<a href="#">58,59</a>
S	1675 (500-1100)	2.15	<a href="#">60,61</a>