



SDI Review Form 1.6

Journal Name:	Journal of Materials Science Research and Reviews
Manuscript Number:	Ms_JMSRR_45546
Title of the Manuscript:	ADSORPTION ENERGIES OF LITHIUM AND SODIUM IONS ON VANADIUM DISULPHIDE: A DFT STUDY.
Type of the Article	Original Research Article

General guideline for Peer Review process:

This journal's peer review policy states that **NO** manuscript should be rejected only on the basis of '**lack of Novelty**', provided the manuscript is scientifically robust and technically sound. To know the complete guideline for Peer Review process, reviewers are requested to visit this link:

(<http://www.sciencedomain.org/page.php?id=sdi-general-editorial-policy#Peer-Review-Guideline>)

PART 1: Review Comments

	Reviewer's comment	Author's comment (if agreed with reviewer, correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)
Compulsory REVISION comments	The authors propose a layered material as an electrode for LI- and Na-based batteries. The authors performed DFT calculations of the adsorption energy of Li and Na ions on a VS₂ monolayer. In my opinion, the topic is interesting and it should be properly worked. Additional comments: 1) The proposed exchange correlation function do not consider dispersion corrections, and probably this will be important in the larger ion proposed in this work (Na). M062X, and M11 functionals should be more appropriated. 2) You calculated adsorption energies for only 1 atom, but your figures show that you studied at least two atoms, why you did not report the second energies? A more complete study should study the adsorption energies as a function of the number of empty available adsorption sites. 3) You did calculation with VASP, but you did not offer any details of the methodology or discussed why the values are different. 4) You did not discuss the obtained values for energy and bond length, also did not compared them with other results.	PBE correlation functions were used because of its standard features for geometry optimisations. After optimizations VS₂ can accommodate more than one Li/Na atoms as shown in figure 3 (c) and (d). The scope of the adsorption energies discussed in the manuscript is limited to one atom. All calculations were done in QUANTUM ESPRESSO code with the details highlighted under computational details. VASP results were reported work done by other researchers as per reference number (20) and (21).

PART 2:

	Reviewer's comment	Author's comment (if agreed with reviewer, correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)
Are there ethical issues in this manuscript?	(If yes, Kindly please write down the ethical issues here in details)	No ethical issues.