Supporting information

Ab Initio Study of 2D h-BAs monolayer: A promising anode material for Alkali-Metal Ion Batteries

N. Khossossi[*a,c], A. Banerjee[*d], Y. Benhouria[a], I. Essaoudi[a,c], A. Ainane[a,b,c], and R. Ahuja[c,d]

[a]*Laboratoire de Physique des Matériaux et Modélisations des Systèmes, (LP2MS), Unité Associée au CNRST-URAC 08, Moulay Ismail University, Faculty of Sciences, Department of Physics, B.P. 11201, Meknes, Morocco*
[b]*Max-Planck-Institut für Physik Complexer Systeme, NöthnitzerStr. 38 D-01187 Dresden, Germany*
[c]*Condensed Matter Theory Group, Department of Physics and Astronomy, Uppsala University, 75120 Uppsala, Sweden*
and
[d]*Applied Materials Physics, Department of Materials and Engineering, Royal Institute of Technology (KTH), S-100 44 Stockholm, Sweden*

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* Corresponding authors. Emails:
n.khossossi@hotmail.com & amitava245@gmail.com

Table S1. The calculated E_A values for all considered adsorption sites, with respect to the vacuum reference states and bulk-metal reference states.

Adsorption Sites	Total Energy of adsorbed state (eV)			Adsorption of alkali-metals on h-BAs monolayer (eV)					
	Li@BAs	Na@BAs	K@BAs	E_A (Li-isolated)	E_A (Li-bulk)	E_A (Na-isolated)	E_A (Na-bulk)	E_A (K-isolated)	E_A (K-bulk)
H-site	-1701,79	-1795,98	-1799,78	-2.393	-0.422	-1.658	-0.322	-1.817	-0.814
T_{As}-site	-1701,76	-1795,97	-1799,78	-1.970	-0.013	-1.490	-0.153	-1.746	-0.743
T_B-site	-1701,75	-1795,96	-1799,77	-1.843	0.113	-1.333	0.003	-1.615	-0.612

Figure S1

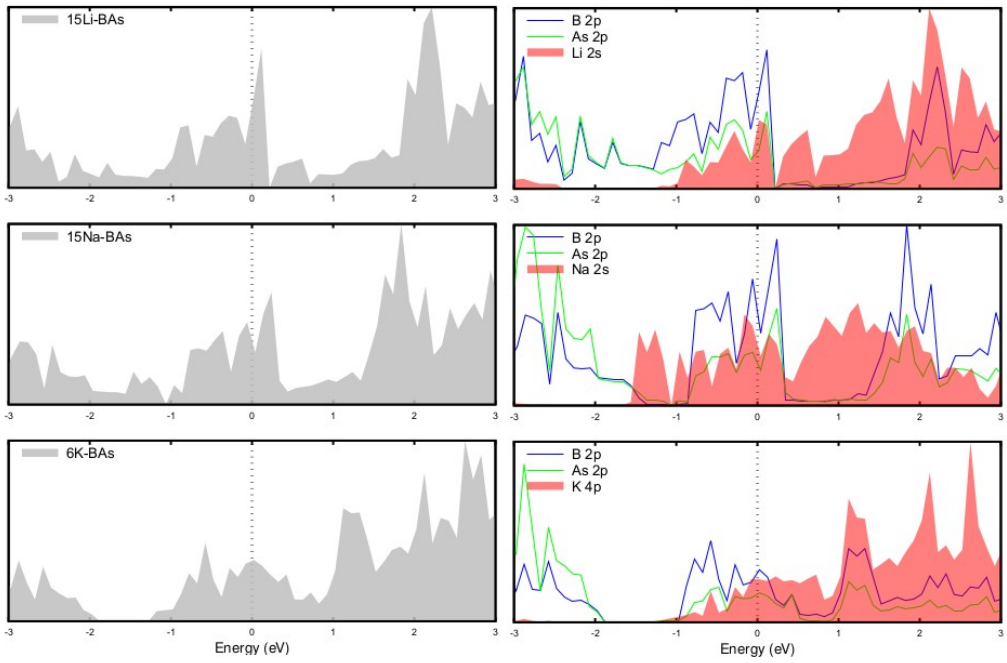

Figure S1. Total and Partial density of states (TDOS & PDOS) of h-BAs monolayer with highest capacity of adatoms. The Fermi levels are set to zero and are indicated by the dashed lines.