# Supporting Information Two-Dimensional Stable Transition Metal Carbides MnC and NbC with Prediction and novel Functionalizations

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August 16, 2018

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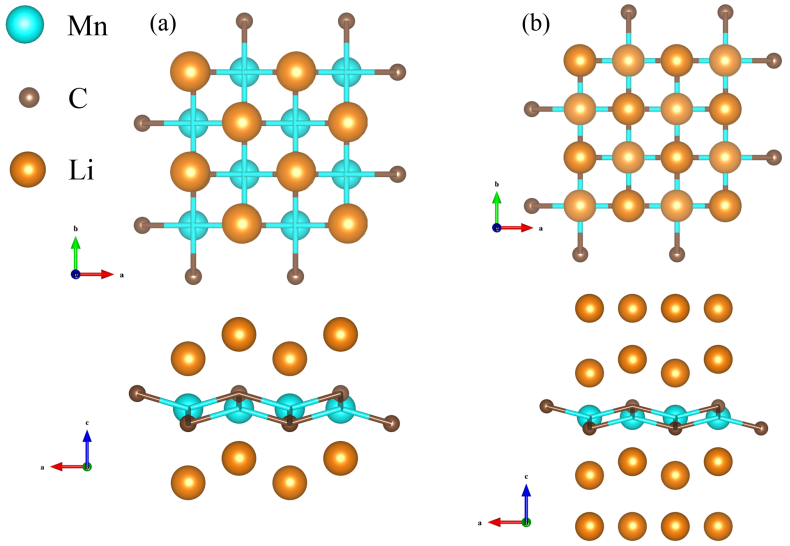


Figure S1: The optimized structures of (a) the adsorption structure of $Mn_8C_8Li_{16}$ (b) the adsorption structure of $Mn_8C_8Li_{32}$.

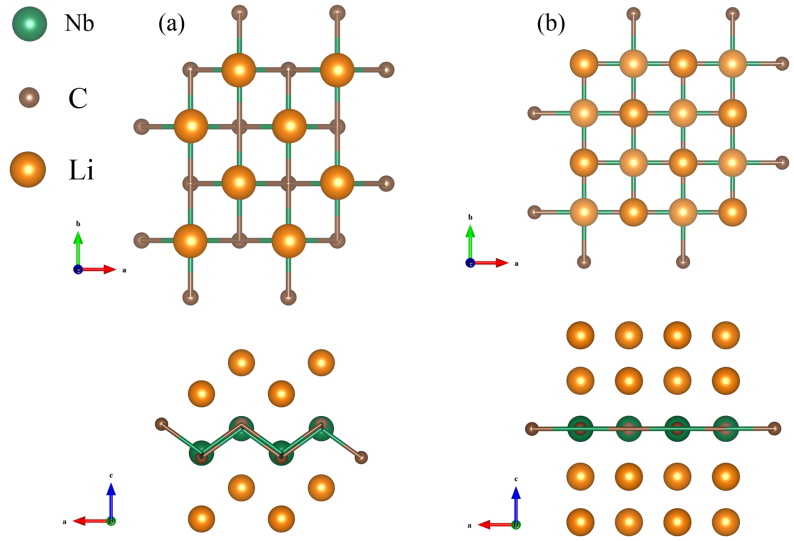


Figure S2: The optimized structures of (a) the adsorption structure of $Nb_8C_8Li_{16}$ (b) the adsorption structure of $Nb_8C_8Li_{32}$.

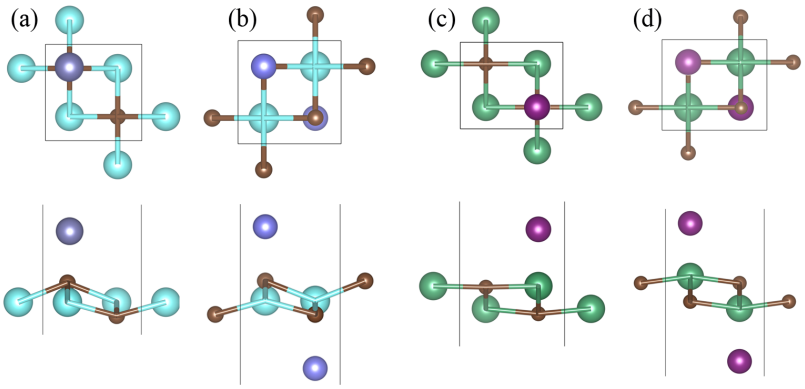


Figure S3: The optimized structures of (a) single surface and (b) double surface passivation by F, Cl, Br, I or O atom of MnC monolayer, and the optimized structures of (c) single surface and (d) double surface passivation by F, Cl, Br or I atom of NbC monolayer.

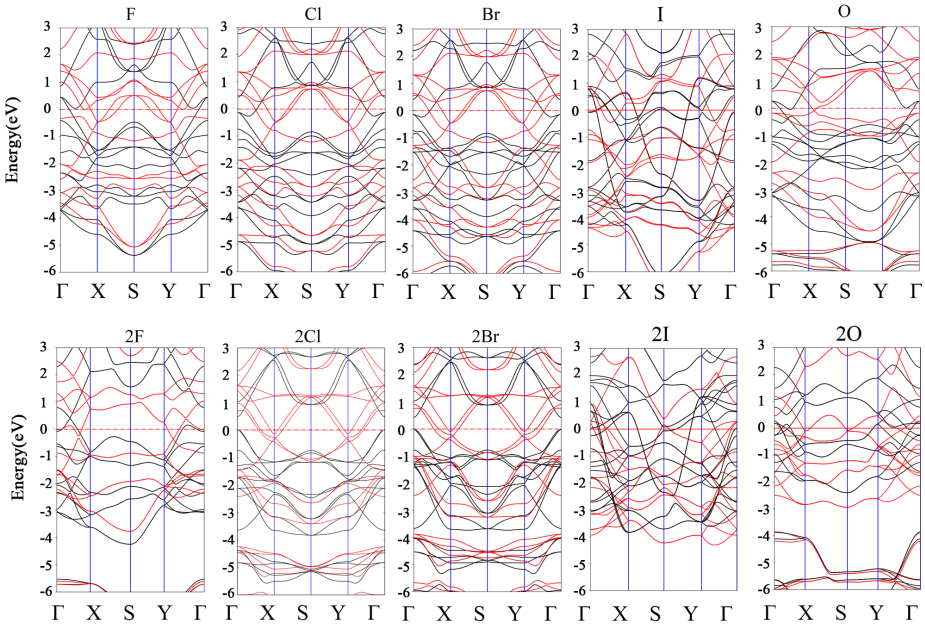


Figure S4: The electronic bands of single surface and double surface passivation by F, Cl, Br, I or O atom of MnC monolayer.

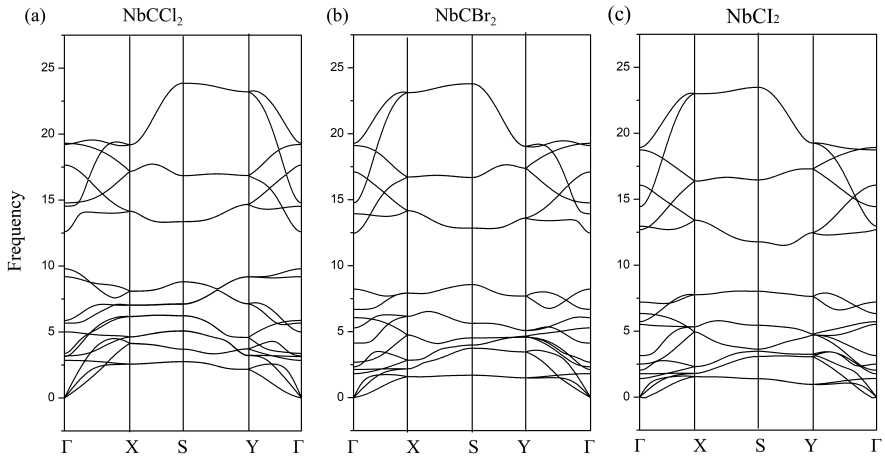


Figure S5: The phonon dispersion of double surface passivation by Cl, Br and I atom of NbC monolayer.

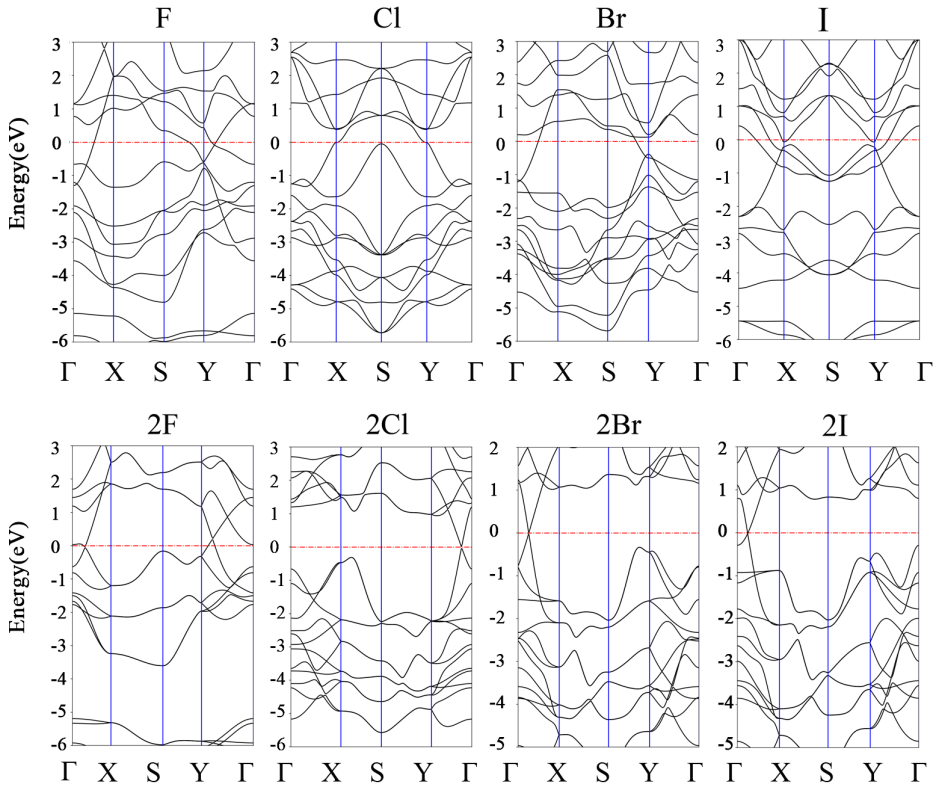


Figure S6: The electronic bands of single surface and double surface passivation by F, Cl, Br or I atom of NbC monolayer.

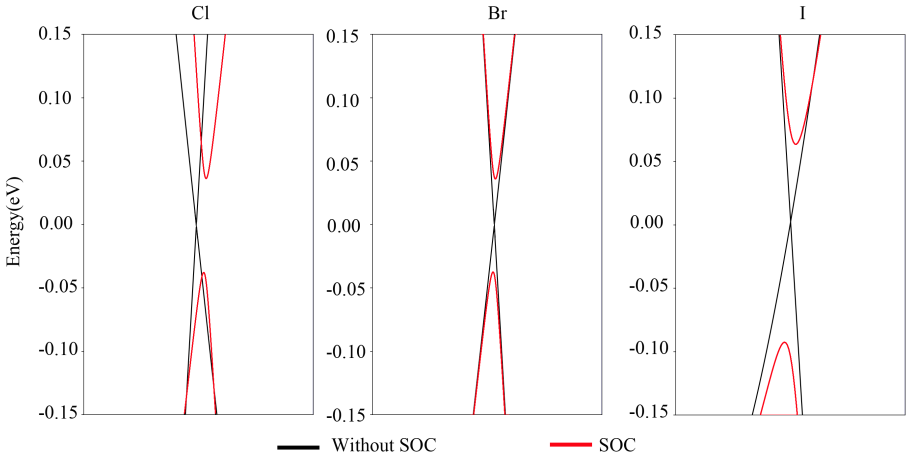


Figure S7: The zoom-in electronic bands of double surface passivation by Cl, Br or I atom of NbC monolayer with and without SOC.