# Enhancing superconductivity in MXenes through hydrogenation 

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## VIBRATIONAL PROPERTIES



Mor $\mathbf{N O}$

| Mor $\mathbf{N H}_{2}$ - Model I |  |
| :---: | :---: |
|  |  |
| Mo ${ }_{2} \mathbf{N H}_{2}-$ Model III | $\mathrm{Mo}_{2} \mathrm{NH}_{2}$ - Model IV |
|  |  |



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## ELECTRONIC BAND STRUCTURES




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FERMI SURFACES



## ELECTRON-PHONON COUPLING

| Mor ${ }_{2}$ | Mor $\mathrm{CH}_{2}$ - Model I |
| :---: | :---: |
|  |  |
| $\mathrm{Mo}_{2} \mathrm{CH}_{2}$ - Model III | $\mathrm{Mo}_{2} \mathrm{CH}_{2}$ - Model IV |
|  |  |


| Mor ${ }^{\text {N }}$ | Mo $\mathbf{N H}_{2}$ - Model I |
| :---: | :---: |
|  |  |
| $\mathbf{M o} \mathbf{N O H}_{\mathbf{2}}$ - Model III | Mo ${ }_{2} \mathbf{N H}_{2}$ - Model IV |
|  |  |



| $\mathrm{W}_{2} \mathrm{~N}$ | $\mathbf{W}_{2} \mathbf{N H}_{2}$ - Model I |
| :---: | :---: |
|  |  |
| $\mathrm{W}_{2} \mathrm{NH}_{2}-$ Model III | $\mathbf{W}_{2} \mathbf{N H}_{2}$ - Model IV |
|  |  |


| $\mathrm{Nb}_{2} \mathrm{C}$ | $\mathrm{Nb}_{2} \mathrm{CH}_{2}$ - Model I |
| :---: | :---: |
|  |  |
| $\mathrm{Nb}_{2} \mathrm{CH}_{2}-$ Model III | $\mathrm{Nb}_{2} \mathrm{CH}_{2}$ - Model IV |
|  |  |

