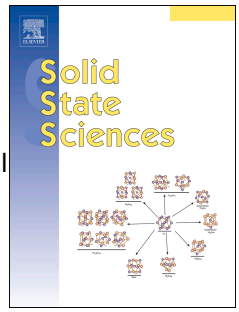

Ab-initio study on the stability, electronic and mechanical properties of transition metal nitrides under external pressure

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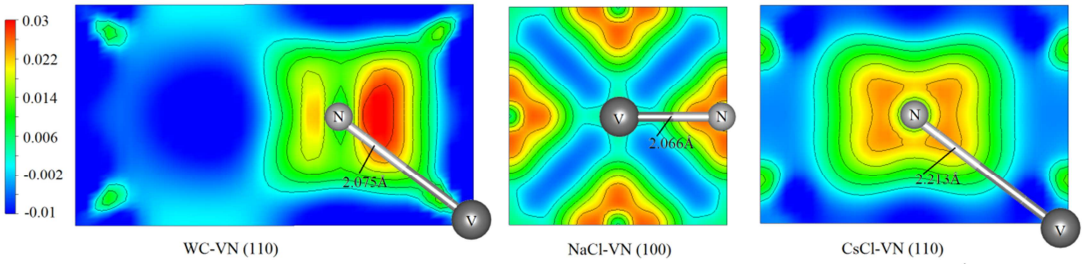
Charge density around TM atoms exhibited directional distribution to N atoms, indicating directional TM−N bond was covalent. The increase with positive value in charge density in the space between TM and N atoms also indicated covalent property of TM−N bond. Charge density at TM atom sites decreased and charge density at N atom sites increased after bonding, indicating ionic property of TM−N bond.



WC-VN (110) NaCl-VN (100) CsCl-VN (110)