Abstract Submitted
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Jahn-Teller induced multiple ferromagnetic exchange interactions in magnetic semiconductors[1] HANNES RAEBIGER, TAKESHI FUJITA, Yokohama National University, Yokohama — Ferromagnetic interactions among $3d$ impurities in compound semiconductors (II-VI, III-V, etc) are usually rationalized via "double exchange", "p-d exchange", and "superexchange" type interactions, which ensue a description of the $3d$ impurity electronic configuration based on host symmetries. Obviously Jahn-Teller distortions break these symmetries and yield completely different, closed shell, electronic configurations for the impurities, which most theories [1] simply describe as magnetically inactive. Nonetheless, such Jahn-Teller distorted $3d$ impurities e.g. in the AlN host exhibit strong short range ferromagnetic interactions. Superexchange models may offer some insight to "closed shell" magnetic interactions, not applicable to the present case, however. We investigate such peculiar magnetic interactions via density-functional calculations, and find that a Jahn-Teller distortion can trigger the formation of a 3d-3d chemical bond that stabilizes ferromagnetism via direct exchange [2], and further facilitates a double exchange type interaction. This multiple exchange is what aligns parallel the spins of e.g. Cr impurities in AlN.

[1] A. Zunger, S. Lany, and H. Raebiger, Physics **3**, 53 (2010).
[2] H. Raebiger, S. Lany, and A. Zunger, PRL **99**, 167203 (2007).

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