

## PC2-4

### Effective model construction of $\text{LaNiO}_2$ ; a possible nickelate analogue of the cuprate superconductors

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Searching for analogues of cuprates has been considered as a possible path toward discovery of new high- $T_c$  superconductors. An infinite layered nickelate  $\text{LaNiO}_2$  has been considered as a possible candidate for such an analogue of cuprates because of its  $d^9$  electron configuration [1,2]. First principles calculations have shown that the  $d_{x^2-y^2}$  bandwidth is narrower than that of the cuprates, and in addition, two electron pockets originating from La 5d orbitals are present. In the present study, in order to study the possibility of superconductivity in  $\text{LaNiO}_2$ , we construct an effective two-orbital model for  $\text{LaNiO}_2$  that takes into account the Ni  $d_{x^2-y^2}$  and  $d_{3z^2-r^2}$  orbitals. Such a model has been constructed for the cuprates by some of the present authors, which lead to a successful reproduction of the experimentally observed trend of  $T_c$  [3]. The on-site interactions are estimated within the random phase approximation [4,5]. The estimation of the interaction parameters for the nickelate shows that the on-site interaction within the  $d_{3z^2-r^2}$  orbital is relatively small due to its hybridization with the La orbitals. The fluctuation exchange study for the two-orbital model of  $\text{LaNiO}_2$  results in d-wave superconductivity similarly to the cuprates, with a somewhat reduced  $T_c$  due to the narrower bandwidth.

[1] V. I. Anisimov, D. Bukhvalov, and T. M. Rice, Phys. Rev. B **59**, 7901 (1999)

[2] K.-W. Lee and W. E. Pickett, Phys. Rev. B **70**, 165109 (2004).

[3] H. Sakakibara *et al.*, Phys. Rev. Lett. **105**, 057003 (2010).

[4] H. Sakakibara *et al.*, J. Phys. Soc. Jpn. **86**, 044714 (2017); H. Sakakibara and T. Kotani, Phys. Rev. B **99**, 195141 (2019).

[5] F. Aryasetiawan *et al.*, Phys. Rev. B **70**, 195104 (2004); S.W. Jang *et al.*, Sci. Rep. **6**, 33397 (2016).

Keywords: Superconductivity, Cuprates, First-principle calculation, Hubbard model