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Possible mechanism of enhanced pairing correlation near dopant oxygen in cuprate MICHIYASU MORI, Japan Atomic Energy Agency, GINIYAT KHALIULLIN, Max-Planck-Institut fur Festkorperforschung, TAKAMI TOHYAMA, Kyoto University, SADAMICHI MAEKAWA, Japan Atomic Energy Agency — Recent experiments on Bi-based cuprate superconductors have revealed an unexpected enhancement of the pairing correlations near the interstitial dopant oxygens. We propose a mechanism by which the dopant oxygens strongly enhance the interaction J locally [1]. We notice that there is a strong covalency between the dopant oxygen and closely located apical oxygens, forming a molecular orbital complex. By considering virtual p-d and d-d charge transitions within the Cu-O-Cu bond that lead to the spin exchange J, we will show that the corresponding excitation energies are screened by the polarization of molecular orbitals hence enhancing J. The effect is greatly amplified due to cooperative response of the spatially extended oxygens complex. We will also show, by an exact diagonalization of the t-J model, that local enhancement of J leads to the spatial variations in density of electronic states observed in STM experiments. Our findings suggest an interesting possibility of quantum-chemistry control of the key interaction J in cuprates.

[1] G. Khaliullin, M. Mori, T. Tohyama, and S. Maekawa, arXiv:1008.0435

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