Abstract Submitted for the MAR17 Meeting of The American Physical Society

Extended Antiferromagnetic Models for Ionic-Covalent Bonding in Crystals CHUN-FENG HUANG, 12nd Patent Division, Intellectual Property Office, Ministry of Economic Affairs, Taipei, Taiwan 106, R.O.C., I.-H. TSAI, Department of Mathematics, National Taiwan University, Taipei, Taiwan 106, R.O.C. — Successful quasiparticle theory has been developed for the correlation effects related to antiferromagnetic (AF) phase such as those in the high-temperature superconductors. In addition, it is well-established how to construct the corresponding two-electron correlated states by considering the half-filled 4-orbital model [1], under which the covalent wavefunction represents the AF state. In this poster, we constructed quasielectrons for chemical bonding by including the ionic part to generalize the AF-type quasielectrons. The Bloch quasi-electron orbitals can be obtained after imposing the periodic condition based on crystal symmetry. [1] Phys. Stat. Sol. (b) 242, No. 2, p.p. 317-321 (2005).

Chun-feng Huang

12nd Patent Division, Intellectual Property Office, Ministry of Economic Affairs, Taipei, Taiwan 106, R.O.C.

Date submitted: 19 Oct 2016 Electronic form version 1.4