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Magnetic model of $BaCuSi_2O_6$ revisited: Bose-Einstein condensation of magnons on a non-frustrated spin lattice[1] ALEXANDER A. TSIRLIN, NICPB, Tallinn, Estonia, VLADIMIR V. MAZURENKO, MARIA V. VALENTYUK, USTU, Ekaterinburg, Russia, RAIVO STERN, NICPB, Tallinn, Estonia — Bose-Einstein condensation (BEC) of magnons remains one of the most intricate collective phenomena observed in quantum magnets. In Han Purple the BEC physics is heavily influenced by structural peculiarities related to the low-temperature structural distortion taking place around 100 K. The crystal structure comprises structural and magnetic dimers forming bilayers, and the BEC transition is formally 2D. Frustrated couplings between the bilayers are believed to be responsible for this effect, because at low enough temperatures the bilayers become decoupled. We challenge this scenario using extensive density-functional (DFT) calculations. We will show that DFT can well reproduce the couplings of $J_A \simeq 50$ K and $J_A \simeq 60$ K in two nonequivalent bilayers. Our calculations also yield a new scenario of the interdimer exchange that takes place between the top site of one dimer and the bottom site of the neighboring dimer rather than top-to-top and bottom-to-bottom. This scenario is verified by INS data and by magnetostructural correlations for the superexchange. The new regime of the interdimer couplings implies that $BaCuSi_2O_6$ lacks any appreciable magnetic frustration, individual bilayers are not decoupled, and other explanations for the 2D BEC physics should be sought

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