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Quantum Computing using Rotational Modes of Dimers KENJI MISHIMA, KOICHI YAMASHITA, Univ. of Tokyo — In this paper, we numerically constructed general-purpose phase-correct global quantum gates by using *inter*molecular rotational modes of two polar molecules coupled by dipole-dipole interaction to encode two qubits and implement the Deutsch-Jozsa algorithm. The calculations were based on the multi-target optimal control theory (MTOCT). The molecular systems we examined were NaCl-NaBr, NaCl-NaCl, and NaBr-NaBr dimer systems. The rotational states in the ground vibrational state of the ground electronic state of these pairs were taken as two qubits. When implementing the Deutsch-Jozsa algorithm by combining these elementary gates, we obtained a maximum probability 97.95 % for NaBr-NaBr system with the interval R=5.0 nm in the repulsive configuration, which is the best performance of the two-state Deutsch-Jozsa algorithm compared with *intra*molecular vibrational-vibrational, vibrational-rotational, and electronic-vibrational qubits reported so far.

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