

# **Supporting Information for “Development of Calculation and Analysis Methods for Dynamic First Hyperpolarizability Based on the Ab Initio Molecular Orbital – Quantum Master Equation Method”**

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## Contents

- jp301213z\_si\_002.pdf:** Movie sequence of  $\rho_{\text{pol}}(\mathbf{r}, t)$  of system **1** shown in Figure 3.
- jp301213z\_si\_003.pdf:** Movie sequence of  $\rho_{\text{pol}}(\mathbf{r}, t)$  of system **2** shown in Figure 3.
- jp301213z\_si\_004.pdf:** Movie sequence of  $\rho_{\text{pol}}(\mathbf{r}, t)$  of system **3** shown in Figure 3.
- jp301213z\_si\_005.pdf:** Movie sequence of SHG response density  $\rho^{(2)}(\mathbf{r}, -2\omega; \omega, \omega) \cos 2\omega t$  of system **1**.
- jp301213z\_si\_006.pdf:** Movie sequence of SHG response density  $\rho^{(2)}(\mathbf{r}, -2\omega; \omega, \omega) \cos 2\omega t$  of system **2**.
- jp301213z\_si\_007.pdf:** Movie sequence of SHG response density  $\rho^{(2)}(\mathbf{r}, -2\omega; \omega, \omega) \cos 2\omega t$  of system **3**.