ЖУРНАЛ СТРУКТУРНОЙ ХИМИИ

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SUPPLEMENTARY MATERIALS TO:

FIRST PRINCIPLES STUDY ON STRUCTURALLY RESOLVED TITANIUM DIOXIDE NANOPARTICLES FUNCTIONALIZED BY ORGANIC LIGANDS

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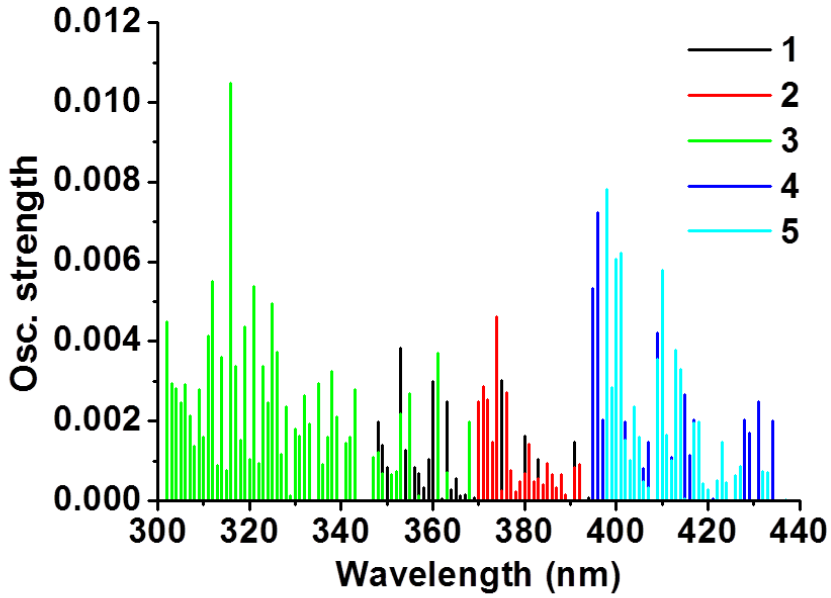

Fig. S1. The optical transitions for **1**-**5** to simulate the UV-vis absorption spectra.

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