Electronic Supplementary Material (ESI) for RSC Advances.

To Unravel Connection between Nonequilibrium and Equilibrium Solvation Dynamics of Tryptophan: Success and Failure of Linear Response Theory of Fluorescence Stokes Shift

Xiaofang Wang,[a] Jirui Guo,[a] Tanping Li,*[a] Zhiyi Wei [b]

[a] School of Physics and Optoelectronic Engineering, Xidian University, Xi'an, 710071, People's Republic of China

[b] Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

*Corresponding author: tpli@xidian.edu.cn

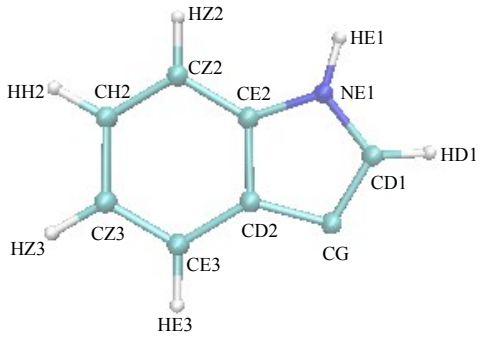

Figure S1: Indole atoms of tryptophan. The spheres in colors represent the carbon (cyan), nitrogen (blue) and hydrogen (white).

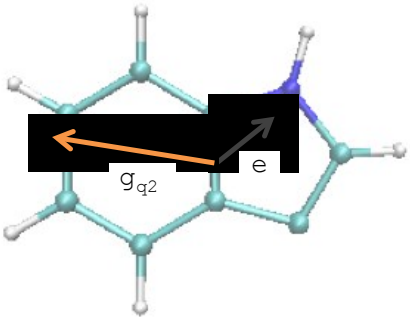

Figure S2: Diople moment of indole for the state g_{q_2} and the excited state e (9.7D and 5.1D respectively) constructed from the partial charges described in Table 1.

Table 1. The simulation parameters for the initial state g, ${}^{g_{T_1}}$, ${}^{g_{q_1}}$, ${}^{g_{q_2}}$ and the excited state (e). Atomic charges of indole are listed. For all the MD simulations, the temperature is set as 298K except for the equilibrium simulation of the state ${}^{g_{T_1}}$, in which the high temperature 353K is taken to acquire a broader configurational sampling.

	atomic charge			
atom	g/ ${}^{g_{T_1}}$	${}^{g_{q_1}}$	${}^{g_{q_2}}$	e
CG	-0.14	-0.095	-0.44	0.01
CD1	-0.1	-0.085	-0.2	-0.05
HD1	0.1	0.1	0.1	0.1
CD2	0	-0.021	0.14	-0.07
NE1	-0.05	0.001	-0.39	0.12
HE1	0.19	0.19	0.19	0.19
CE2	0	0.003	-0.02	0.01
CE3	-0.1	-0.139	0.16	-0.23
HE3	0.1	0.1	0.1	0.1
CZ2	-0.1	-0.139	0.16	-0.23
HZ2	0.1	0.1	0.1	0.1
CZ3	-0.1	-0.097	-0.12	-0.09
HZ3	0.1	0.1	0.1	0.1
CH2	-0.1	-0.118	0.02	-0.16
HH2	0.1	0.1	0.1	0.1