

Correction to "Non-Gaussian Statistics and Nanosecond Dynamics of Electrostatic Fluctuations Affecting Optical Transitions in Proteins"

Daniel R. Martin and Dmitry V. Matyushov*

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The originally published Figure 5 contained a point at 240 K significantly deviating from the trend following from all

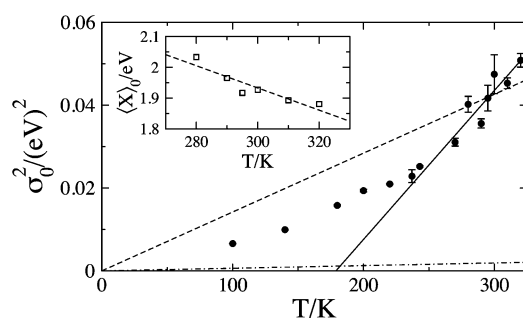


Figure 5. Temperature dependence of the variance of the donor–acceptor energy gap from NVT MD simulations in the S0 state (points, error bars are equal to the point size at lower temperatures). The solid line is the linear fit of the high-temperature portion of the simulation data, and the dashed line is the fit of the same data to the fluctuation–dissipation theorem (FDT), crossing zero at $T = 0$. The dash-dotted line is the prediction of the linear response/FDT, $\sigma_0^2 = 2\lambda^{\text{St}}k_{\text{B}}T$, with λ^{St} taken at 300 K. The inset shows the temperature dependence of the average ground-excited transition energy, $\langle X \rangle_0$. The dashed line in the inset is a linear fit through the simulation points.

other simulated points. The 100 ns long simulation trajectory, used to produce that data point, was later extended to 150 ns, with no change in the value of the spectral width. To check whether the spike is responsible for a physically significant singular behavior, two additional molecular dynamics simulations, at 237 and 243 K, were attempted. The results of both simulations, each 100 ns long, fell on the expected trend. The revised figure therefore has the 240 K point removed and two new points, at 237 and 243 K, added.