

## Errata: Improved tangent estimate in the nudged elastic band method for finding minimum energy paths and saddle points

The equation (A1) in the appendix

$$\begin{aligned}a_i &= \frac{2V_{i+1} - V_i}{R^3} - \frac{F_i + F_{i+1}}{R^2} \\b_i &= \frac{3V_{i+1} - V_i}{R^2} + \frac{2F_i + F_{i+1}}{R} \\c_i &= -F_i \\d_i &= V_i\end{aligned}$$

should be

$$\begin{aligned}a_i &= \frac{-2(V_{i+1} - V_i)}{R^3} - \frac{F_i + F_{i+1}}{R^2} \\b_i &= \frac{3(V_{i+1} - V_i)}{R^2} + \frac{2F_i + F_{i+1}}{R} \\c_i &= -F_i \\d_i &= V_i.\end{aligned}$$

Thanks to Prof. Ju Li for finding this error, and Egill Skúlason for correcting this Erratum.