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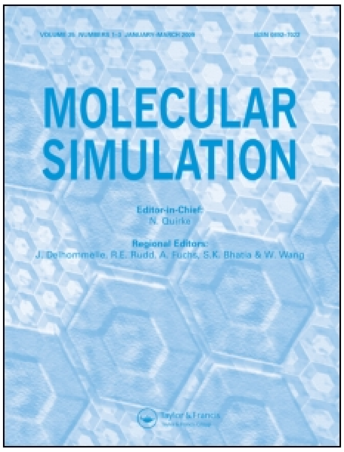

## Molecular Simulation

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# Nearest neighbour considerations in Stillinger-Weber type potentials for diamond

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# NEAREST NEIGHBOUR CONSIDERATIONS IN STILLINGER–WEBER TYPE POTENTIALS FOR DIAMOND

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Results of a preliminary investigation into the effect of varying the interaction cutoff on the bulk properties of diamond using a Stillinger–Weber (SW) type potential for C (Diamond) are presented. The interaction cutoff is varied over a range that includes and excludes the second-nearest neighbours. Whilst the original SW potential for silicon only included first-nearest neighbours inside the interaction cut-off, subsequent parameterizations for carbon (diamond) have also included second-nearest neighbours. Elastic and vibration properties of diamond were calculated over a range of cutoff distances used and the results show that certain lattice properties exhibit an approximately linear dependence on the interaction cut-off.

*Keywords*: Interatomic potential; Stillinger–Weber potential; Diamond; Nearest-neighbour interactions; Elastic constants; Phonon modes

## INTRODUCTION

With the advent of increased computational resources being made available in the scientific community, the computational study of large atomic and molecular systems is becoming more common place. A widely used potential for describing interactions in covalent, tetrahedrally bonded systems is the empirical potential devised by Stillinger and Weber (SW) in 1985 [1], which was first applied to

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silicon. This potential has been successfully applied to calculate the bulk and surface properties of Si [2–4], Ge [5], Si–Ge alloys [6], Si–F [7] and Si–H [8].

Comparative studies of empirical interatomic potentials for silicon, such as the investigation by Balamane [9], have shown that the SW potential compares very well with the alternative empirical potentials in predicting bulk point defects energies, elastic constants, phonon modes and surface reconstruction. These alternative empirical potentials include PTHT [10], Biswas and Hamann (BH) [11], Dodson [12], Tersoff [13] and Bazant and Kaxiras [14]. Table I shows the comparison of results for a small selection of mechanical properties and potentials given in the Balamane study.

The comparative study by Balamane shows that the SW potential gives an excellent description of the physical properties of FCC (Diamond) silicon. Like silicon, carbon is also represented by a number of empirical potentials such as those of Tersoff [15], Marks [16], Brenner [17] and SW [18,19]. It is well known that carbon can exist in a number of bonding forms at room temperature and pressure and for certain computational studies, such as modelling CVD of diamond thin films, it is essential that an empirical potential be able to accurately model sp, $sp^2$ and $sp^3$ bonded carbon. The "bond order" potentials of Tersoff [15], Marks [16], Brenner [17] are able to model all these forms of carbon where the SW potential is not. However, if only $sp^3$ bonded carbon clusters are under consideration, as might be found in a diamondoid nano-structures [20], the Balamane study indicates that the SW potential should compare well with these "bond order" potentials. Table II contains a comparison of the elastic constants and the bulk modulus for carbon (diamond) for the Brenner, Tersoff and SW potentials, along with the experimental values and shows that the SW potential is a reasonable choice for the description of $sp^3$ bonded carbon. In addition the SW potential allows for efficient numerical implementation and parallelization, and

TABLE I Comparison of elastic constant and bulk moduli (in Mbars) and phonon frequencies (in THz) for FCC (Diamond) Si; for the SW, BH, and Tersoff empirical potentials (from Balamane *et al.* [9])

| *Property* | *Experiment* | *SW* | *BH* | *Tersoff II* | *Tersoff III* |
|---|---|---|---|---|---|
| $C_{11}$ | 1.67* | 1.616 | 2.042 | 1.217 | 1.425 |
| $C_{12}$ | 0.65* | 0.816 | 1.517 | 0.858 | 0.754 |
| $C_{44}$ | 0.81* | 0.603 | 0.451 | 0.103 | 0.690 |
| B | 0.99* | 1.083 | 1.692 | 0.98 | 0.98 |
| LTO($\Gamma$) | 15.3† | 18.1 | 16 | 16.5 | 16 |
| TA($X$) | 4.4† | 6.7 | 5.6 | 2.7 | 9 |
| TO($X$) | 13.9† | 15.9 | 14.5 | 15.3 | 16 |
| LAO($X$) | 12.3† | 13.1 | 12.2 | 11.7 | 12 |

* Ref. [30].
† Ref. [31].

TABLE II Comparison of elastic constants and Bulk Modulus of Carbon (diamond) in Mbars, for the SW parameterisation used in this study, the SW diamond potential of Mahon and Pailthorpe [MP] [18], Brenner [unpublished] and Tersoff [15] potentials, with experiment [32]

| *Property* | *Experiment* | *SW* | *SW [MP]* | *Brenner* | *Marks* | *Tersoff* |
|---|---|---|---|---|---|---|
| $C_{11}$ | 10.76 | 11.47 | 9.72 | 10.7 | 10.57 | 10.9 |
| $C_{12}$ | 1.25 | 1.21 | 0.60 | 1.2 | 0.99 | 1.2 |
| $C_{44}$ | 5.77 | 5.2 | 4.3 | 7.2 | 4.7 | 6.4 |
| Bulk Modulus | 4.42 | 4.63 | 3.64 | 4.37 | 4.18 | 4.43 |

these features make the SW potential an excellent candidate for the modelling of large tetrahedral covalent bonded structures of the order of tens or hundreds of thousands of particles.

A significant factor in the computational performance of the SW (or any) empirical potential is the effective interaction distance. For example, an interaction distance that includes second nearest neighbours does significantly affect the size of a system, which can be simulated. For tetrahedral bonded structures, their inclusion increases the number of two body interactions (for a particular atom) from 4 to 16 and the number of three body interactions (for the same atom) from 12 to 240. The purpose of this study was to determine how the calculated bulk elastic and vibrational properties of diamond changed with the interaction cutoff and in particular to determine the affect of exclusion or inclusion of second nearest neighbours on those properties.

## THE STILLINGER–WEBER POTENTIAL

The original SW potential is written as a sum of two-body and three-body interaction terms for an $N$ atom system,

$$\frac{U_N}{\varepsilon} = \sum_{i<j} U^{(2)}(r_{ij}/\sigma) + \sum_{i<j<k} U^{(3)}(r_i/\sigma,\ r_j/\sigma,\ r_k/\sigma), \tag{1}$$

where $U^{(2)}$ and $U^{(3)}$ are the two-body and three-body interaction terms, respectively (in reduced units), expressed as:

$$U^{(2)}(r_{ij}) = \begin{cases} A(Br_{ij}^{-4} - 1)\exp\{(r_{ij} - a)^{-1}\} & r < a \\ 0 & r \geq a \end{cases} \tag{2}$$

and,

$$U^{(3)}(r_i, r_j, r_k) = h(r_{ij}, r_{ik}, \theta_{jik}) + h(r_{ji}, r_{jk}, \theta_{ijk}) + h(r_{ki}, r_{kj}, \theta_{ikj}) \tag{3}$$

where,

$$h(r_{ij}, r_{ik}, \theta_{jik}) = \lambda \exp\{\gamma(r_{ij} - a)^{-1} + \gamma(r_{ik} - a)^{-1}\}(\cos\theta_{jik} - \cos\theta_t)^2 \qquad (4)$$

In Eqs. (2)–(4) the distances are in reduced units and $h(r_{ji}, r_{jk}, \theta_{ijk})$ and $h(r_{ki}, r_{kj}, \theta_{ikj})$ have the same functional form as $h(r_{ij}, r_{ik}, \theta_{jik})$. The parameters $\epsilon$ and $\sigma$ are the energy and length scaling parameters, respectively and the parameters $A$, $B$, $\lambda$, $\gamma$, $a$, $\epsilon$ and $\sigma$ comprise the fitting parameters in the SW potential and are fitted to *ab initio* bond-stretch and bond-bend energy data or experimental results or both [1,4,8,18,19]. A central feature of the original SW potential is that the three-body term exclusively favours tetrahedral bonding (i.e. $\cos\theta_t = -1/3$). Hence, as stated in the previous section, in this form the potential is not suitable for modelling non-tetrahedral systems such as graphite.

A SW parameterisation for carbon (diamond) was first produced by Pailthorpe and Mahon [18] who used *ab initio* methods to determine the fitting parameters. In this study, we have used a new parameterisation (also based on quantum mechanical *ab initio* calculations) for diamond-like carbon, which gives general elastic constants that are closer to experiment [19] than the original C paramerisation. The values of the fitting parameters in this new parameterisation

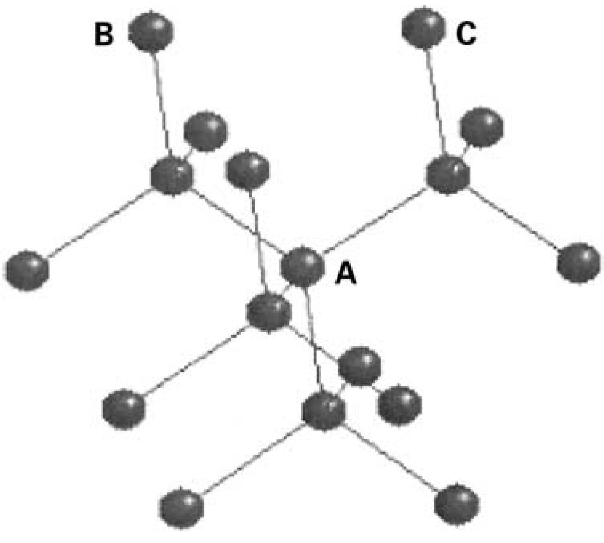

FIGURE 1 Second-nearest neighbour group labelling atoms *A*, *B* and *C*.

are:

$$A = 5.3789794, \quad B = 0.5933864, \quad \lambda = 26.19934, \quad \gamma = 1.055116,$$

$$a = 1.846285, \quad \varepsilon(\text{eV}) = 3.551, \quad \sigma(\text{Å}) = 1.368$$

While the original SW potential for silicon included only the first-nearest neighbours, both carbon parameterisations include the second-nearest neighbours in the interaction, in order to obtain significant (2 × 1) reconstruction of the (100) diamond surface and (1 × 1) and (2 × 1) reconstruction of the (111) diamond surface [21] in reasonable simulation time. However, extending the interaction cut-off to include second-nearest neighbours does result in certain interactions which are *not* correctly modelled by the SW three-body energy term $U^{(3)}$ when $\theta_t = 109.47°$ is used in the angular term. We illustrate this point in Fig. 1, which labels two (second nearest) neighbours to a particular central atom.

If the interaction cutoff *a* in the SW potential allows for the inclusion of second nearest neighbour interactions then the triplet interaction of A with B and C will contribute to the SW three body energy. Although the SW three-body term is defined in terms of the ideal tetrahedral angle, the angle *BAC* is equilateral, and therefore this contribution to the calculated, three body, energy will not be accurate. Closer inspection of diamond lattice structure will also reveal that there are a number of possible 2nn–2nn–2nn (where 2nn denotes second nearest neighbour) triplet combinations which are not tetrahedrally coordinated. To determine whether their combined erroneous contributions to the three-body energy is significant (in the sense that they lead to inaccurate calculations of mechanical properties) we have calculated various bulk properties as a function the interaction cutoff length in the SW potential.

The effects of first-nearest and second-nearest neighbour interactions have been considered via a minor modification to the SW terms that allows inclusion or exclusion of the second-nearest neighbours to be controlled explicitly. This modification entails the introduction of an additional parameter $\alpha$ in the two-body and three-body terms, such that:

$$U^{(2)}(r_{ij}) = \begin{cases} A(Br_{ij}^{-4} - 1)\exp\{(r_{ij} - \alpha a)^{-1}\} & r < \alpha a \\ 0 & r \geq \alpha a \end{cases} \tag{5}$$

and,

$$h(r_{ij}, r_{ik}, \theta_{jik}) = \lambda \exp\{\gamma(r_{ij} - \alpha a)^{-1} + \gamma(r_{ik} - \alpha a)^{-1}\}(\cos\theta_{jik} - \cos\theta_t)^2 \tag{6}$$

with similar forms for $h(r_{ji}, r_{jk}, \theta_{ijk})$ and $h(r_{ki}, r_{kj}, \theta_{ikj})$. Here, the product $a\alpha$ denotes the interaction cut-off in reduced units. Experimental values for the first and second nearest neighbour distances of diamond are 1.5445 and 2.5221 Å, respectively (corresponding to $\alpha = 0.6115$ and $\alpha = 0.9986$). Here $\alpha$ operates as a switch controlling the inclusion or exclusion of the second-nearest neighbours in the potential. Equation (7) shows the values of $\alpha$ which correspond to the first and second nearest neighbour interaction range used in this study.

$$\alpha = \begin{cases} 0.974931 & \text{First-nearest neighbour minimum} \\ 0.993587 & \text{First-nearest neighbour maximum} \\ 1 & \text{Second-nearest neighbour minimum} \\ 1.029094 & \text{Second-nearest neighbour maximum} \end{cases} \tag{7}$$

For each simulation undertaken, only the value of $\alpha$ was varied. All other SW fitting parameters were given by their above stated values.

## RESULTS AND DISCUSSION

Table III gives the calculated elastic constants, bulk modulus, Poisson's ratio, *X*-point and $\Gamma$-point phonon mode frequencies for the various interaction cutoffs. The elastic constants $C_{11}$, $C_{12}$ and $C_{44}$ were calculated using the method of Cowley [22]. The bulk modulus (B) and [100] Poisson's ratio $\sigma_{[100]}$ were subsequently evaluated using Eqs. (8) and (9).

TABLE III Elastic (in Mbars) and vibrational properties (in THz) calculated using the respective values of $\alpha$. Note that Cut-off 2 is just below the second-nearest neighbour distance, and Cut-off 3 is just above

| *Property* | *Experiment* | *Cut-off 1* | *Cut-off 2* | *Cut-off 3* | *Cut-off 4* |
|---|---|---|---|---|---|
| Cut-off(Å) | N/A | 1.80 | 1.834448 | 1.846285 | 1.90 |
| $\alpha$ | N/A | 0.974931 | 0.993587 | 1.000000 | 1.029094 |
| $C_{11}$ | 10.76* | 10.08 | 11.11 | 11.47 | 13.15 |
| $C_{12}$ | 1.25* | 1.67 | 1.33 | 1.21 | 0.593 |
| $C_{44}$ | 5.77* | 4.59 | 5.03 | 5.2 | 5.79 |
| B | 4.42† | 4.48 | 4.59 | 4.63 | 4.78 |
| $\sigma_{[100]}$ | 0.1* | 0.14 | 0.11 | 0.095 | 0.043 |
| LTO($\Gamma$) | 39.9‡ | 53.7 | 55.8 | 56.5 | 59.7 |
| TA(X) | 24.1‡ | 27.4 | 29.1 | 29.7 | 32.8 |
| TO(X) | 32.3‡ | 46.2 | 48.0 | 48.5 | 51.4 |
| LAO(X) | 35.8‡ | 40.0 | 41.8 | 42.4 | 45.1 |

* Ref.[32].
† Ref.[26].
‡ Ref.[33].

$$B = \frac{1}{3}(C_{11} + 2C_{12}) \tag{8}$$

$$\sigma_{[100]} = \frac{C_{12}}{C_{11} + C_{12}} \tag{9}$$

The *X*-point and *Γ*-point first-order phonon modes were calculated using the Frozen Phonon Method [23].

From Table III it can be seen that the cutoff which gives the best results over the range of properties considered is probably $\alpha = 1$ (which corresponds to our original parameterisation). Interestingly $\alpha = 1$ includes the second nearest neighbour contributions. This indicates that the erroneous second nearest neighbour energy contributions to the three-body energy are probably small. Figures 2 and 3 give the elastic constant and phonon mode results for values of $\alpha a$ ranging 1.80 (cutoff 1) to 1.90 (cutoff 4). The results show the elastic constants and frozen phonon modes were found to be approximately linearly dependent upon the interaction cutoff distance.

If we compare the results of cut-off 2 (the maximum first nearest neighbour interaction distance) and cut-off 3 the (minimum second nearest neighbour interaction distance) from Table III we are able to gauge the effect of exclusion of second nearest neighbours on the elastic and vibration properties of diamond. For these respective values of $\alpha$ there is only a relatively small difference in the overall accuracy in the description of the elastic and vibrational properties. This

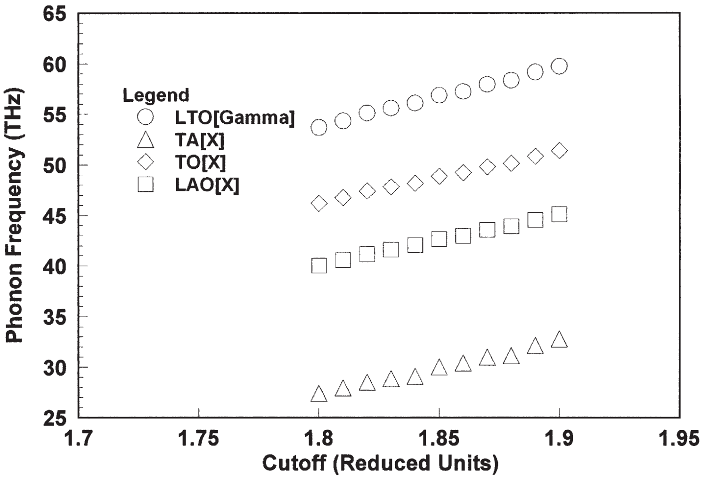

FIGURE 2 Linear dependence of the frozen phonon frequencies on the interaction cut-off $\alpha a$ (in reduced units).

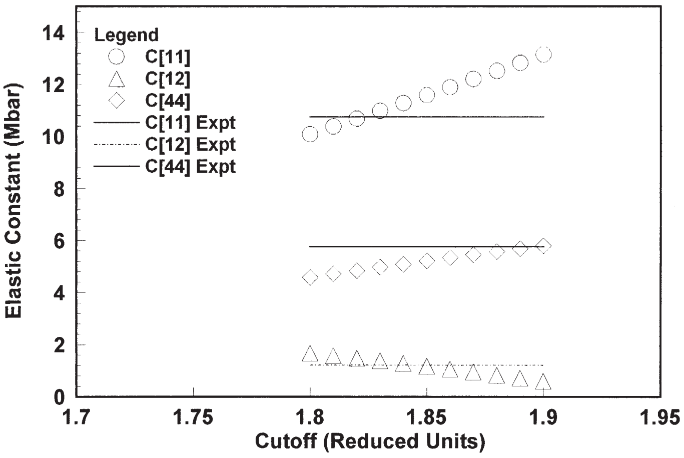

FIGURE 3 Linear dependence of the elastic constants on the interaction cut-off $\alpha a$ (in reduced units).

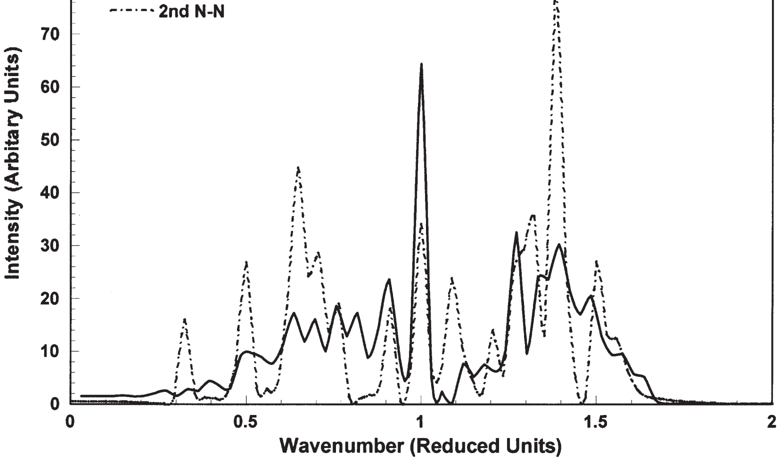

FIGURE 4 VDOS for bulk diamond at 300 K, for $\alpha = 0.993587$ giving only first-nearest neighbours (1st N–N), and $\alpha = 1$ including first and second-nearest neighbours (2nd N–N).

indicates that an accurate re-parameterisation to include only first nearest neighbours may be possible, however, a more detailed study is required for this to be fully determined and such a study is currently being undertaken.

The Vibrational Density of States (VDOS) for bulk diamond was also calculated using first-nearest neighbours ($\alpha = 0.993587$) and second-nearest neighbours ($\alpha = 1$) and is shown in Fig. 4.

The VDOS was determined by calculating the velocity autocorrelation function during an MD simulation [24] and then performing a Fourier transform to calculate the VDOS spectrum [25]. In Fig. 4, the VDOS frequencies are given in reduced wavenumber units and scaled by the $\Gamma$-point wavenumber in each case for comparison purposes. The figure shows the exclusion of the second-nearest neighbours reduces the prevalence of the (IR active) second-order spectrum in the calculated vibrational density of states. This dependence has been previously reported by Windl *et al.* in 1993 [26] as being a direct result of the weighting of the Overtone and Combination spectra by the appropriate polarisability coefficients; which depend upon the contributions of the second-nearest neighbour in the diamond lattice.

## COMPUTATIONAL CONSIDERATIONS

Molecular dynamics simulations are dominated by force calculations (our profiling indicates 80–90%), and thus it is to be expected that the inclusion of second-nearest neighbours in force calculations will increase computational requirements. This is a direct implication of the fact that a carbon atom may be involved in either 4 or 12 two-body interactions depending on the inclusion or exclusion of second-nearest neighbours.

Similarly, an atom may be involved in 12 or 240 three-body interactions depending on the inclusion or exclusion of second-nearest neighbours. The computational impact of inclusion or exclusion of second nearest neighbours was measured using timing experiments in which we measured the CPU time taken to simulate various sized systems. Here results for three finite systems (structures) and one infinite (bulk) system are reported. The finite structures are diamond cubes of approximate sizes 1, 8, and 64 $\mathrm{nm}^3$. These structures are being used in an ongoing molecular dynamics investigation of nanostructures [27]. The infinite system uses periodic boundary conditions with a primary cell of 1000 atoms, giving a cube of 125 unit-cells. The timing experiments were conducted using a Compaq DS10 Alphaserver with a 466 MHz 21264 CPU and 256 MB of main memory running Alpha Linux. Measurements were made of CPU time for a 1000 time-step simulation of the systems at 300 K. Second-nearest neighbours were

TABLE IV Timing experiment results, in CPU seconds

| *System type* | *System size* | *Atoms* | *Inclusion (s)* | *Exclusion (s)* | *Factor* |
|---|---|---|---|---|---|
| Finite | 1 nm$^3$ | 259 | 17.7 | 6.3 | 2.8 |
| Finite | 8 nm$^3$ | 1798 | 193.2 | 72.8 | 2.7 |
| Finite | 64 nm$^3$ | 13324 | 1858.1 | 394.4 | 4.7 |
| Infinite | 125 unit cells | 1000 | 222.2 | 53.5 | 4.1 |

included by setting $\alpha = 1.01$ and excluded by setting $\alpha = 0.99$. Our molecular dynamics implementation is written in Fortran 90 and was compiled with the Compaq Fortran for Linux compiler version V1.0–920 with optimisation at the (default) $-$O4 level. Neighbour lists together with a grid data structure are used to improve performance [28,29]. Results of the timing experiments are given in Table IV. A performance factor in the range of approximately 2–5 difference for the test systems was observed, with the trend to larger performance factors for larger systems, including the infinite system, due to a surface-to-volume ratio effect.

## CONCLUSION

This study has investigated the effect of varying the interaction cutoff of the bulk elastic and vibrational properties of diamond using the SW potential. It was found that the calculated elastic constants and phonon modes were approximately linearly dependent on the interaction distance over the range considered. In particular, it was found that the exclusion of second nearest neighbours did not significantly affect the accuracy of the calculated properties (when compared to experiment). It was found that the exclusion of second nearest neighbours decreased the computational (CPU) time required for a MD run by a factor of 2–5, depending on the system size.

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