Comment on Mostar Indices of SiO_2 Nanostructures and Melem Chain Nanostructures

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The recently reported results by Akhter et al. [International Journal of Quantum Chemistry, **121**(5) (2021) e26520] on the Mostar indices of SiO_2 nanosheet, C_8 layer structure and melem chains are flawed and in error. We establish here that this is due to the incorrect technique employed by Akhter et al., and various computational flaws in their work. In this comment, we correct all of the erroneous results by employing the correct mathematical methods and validate the present results with independent computational programming methods.

1 Introduction

A silicon dioxide unit cell is comprised of an octahedron by connecting the SiO_2 molecular units containing one silicon atom bonded to four oxygen atoms. When these octagon units are joined together we obtain a silicon dioxide nanosheet and a C_8 layer structure obtained by removing all the pendant bonds as shown in Figures 1 and 2. Melem unit cell consists of three hexagons arranged in a triangular manner and a unit cell of the melem structure with hydrogen atoms is given in Figure 3a and without hydrogen atoms in Figure 3b. Recently [1], vertex, edge and total versions of the Mostar index have been computed for SiO_2 nanosheet, C_8 layer structure and melem chains. We show here that all of the computed results

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in [1] are incorrect due to inappropriate mathematical techniques used for the SiO_2 nanostructures and computational as well as constructional flaws on melem chains. Furthermore, our analytical results were independantly validated using TopoChemie-2020 package for the computation of these indices [2].

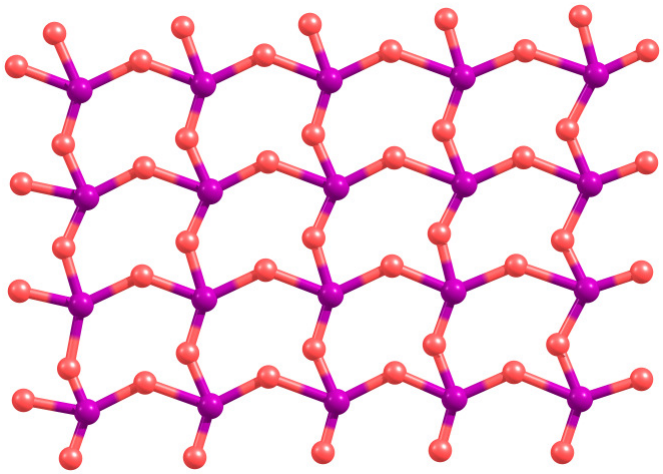


Figure 1: SiO_2 nanosheet of dimension $[3, 4]$

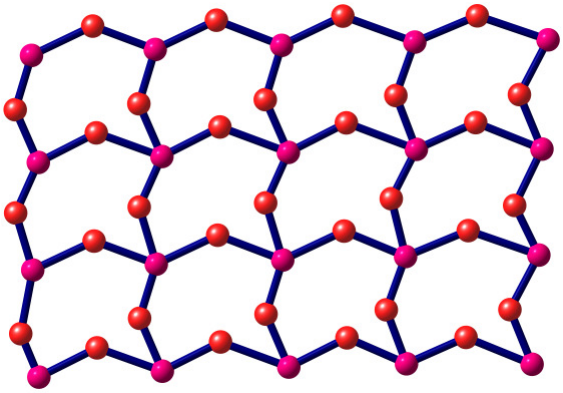
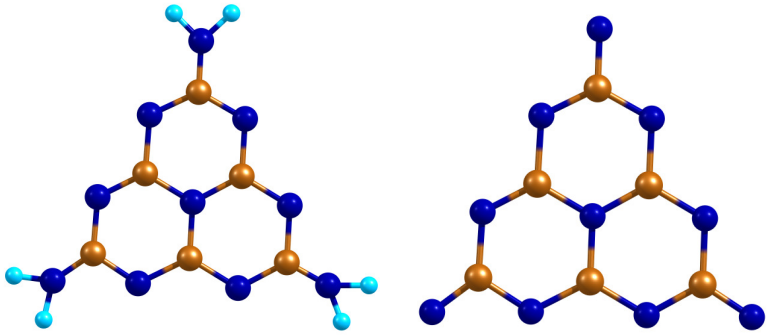


Figure 2: C_8 layer of dimension $[3, 4]$



(a) (b)

Figure 3: Unit cell of melem structure (a) with hydrogens, (b) without hydrogens

In order to proceed with the mathematical definitions of Mostar indices [4, 5], we define the various graph-theoretical terms employed in our study. A graph G consisting of vertex set $V(G)$ and edge set $E(G)$ defines the open neighborhood $N_G(v)$ as the set of vertices adjacent to v. For any two vertices $u, v \in V(G)$, the distance between them denoted as $d_G(u, v)$ is the number of edges in a shortest path from the vertex u to v. The shortest distance between the vertex u and the edge $f = xy \in E(G)$ is defined as $d_G(u, f) = \min\{d_G(u, x), d_G(u, y)\}$. The cardinalities of the bond-additive sets of an edge $h = uv$ are defined in the following.

(i) $n_u(h|G) = |\{x \in V(G) : \ d_G(u, x) < d_G(v, x)\}|$.

(ii) $m_u(h|G) = |\{f \in E(G) : \ d_G(u, f) < d_G(v, f)\}|$.

(iii) $t_u(h|G) = n_u(h|G) + m_u(h|G)$.

(iv) $n_v(h|G)$, $m_v(h|G)$ and $t_v(h|G)$ are analogous to (i)-(iii).

A graph G with strength-weighted functions (SW_V, SW_E) assigned to the vertex set $V(G)$ and edge set $E(G)$ is a strength-weighted graph [3] $G_{sw} = (G, SW_V, SW_E)$, where SW_V is the pair (w_v, s_v) of a vertex weight function $w_v : V(G) \to \mathbb{R}_0^+$ and a strength function $s_v : V(G) \to \mathbb{R}_0^+$, while SW_E is the pair (w_e, s_e) of an edge weight function $w_e : E(G) \to \mathbb{R}_0^+$ and a strength function $s_e : E(G) \to \mathbb{R}_0^+$. To study the Mostar indices, the function w_e does not require and henceforth $G_{sw} = (G, SW_V, s_e)$. The distance function of the strength-weighted graph G_{sw} remains the same as in the graph graph G, while the bond additive set parameters of a vertex u and an edge $h = uv$ are defined as follows.

(i) $n_u(h|G_{sw}) = \sum_{x \in N_u(h|G_{sw})} w_v(x)$.

(ii) $m_u(h|G_{sw}) = \sum_{x \in N_u(h|G_{sw})} s_v(x) + \sum_{f \in M_u(h|G_{sw})} s_e(f)$.

(iii) $t_u(h|G_{sw}) = n_u(h|G_{sw}) + m_u(h|G_{sw})$.

The vertex, edge and total versions of the Mostar index are defined in the following for G and for the strength-weighted graph G_{sw}, each absolute measure is multiplied with the corresponding edge strength value.

- $Mo_v(G) \ = \sum_{h=uv \in E(G)} \big|n_u(h|G) - n_v(h|G)\big|$.
- $Mo_e(G) \ = \sum_{h=uv \in E(G)} \big|m_u(h|G) - m_v(h|G)\big|$.
- $Mo_t(G) \ = \sum_{h=uv \in E(G)} \big|t_u(h|G) - t_v(h|G)\big|$.

Furthermore, it should be noted that $Mo_t(G) = Mo_v(G) + Mo_e(G)$ whenever $n_u(h|G) \geq n_v(h|G)$ and $m_u(h|G) \geq m_v(h|G)$ or $n_u(h|G) \leq n_v(h|G)$ and $m_u(h|G) \leq m_v(h|G)$ for every edge h in G. On the other hand, $Mo_t(G) \neq Mo_v(G) + Mo_e(G)$ whenever $n_u(h|G) > n_v(h|G)$ and $m_u(h|G) < m_v(h|G)$ or $n_u(h|G) < n_v(h|G)$ and $m_u(h|G) > m_v(h|G)$ for some h in G which is possible when the graph is clustered as shown in Figure 4.

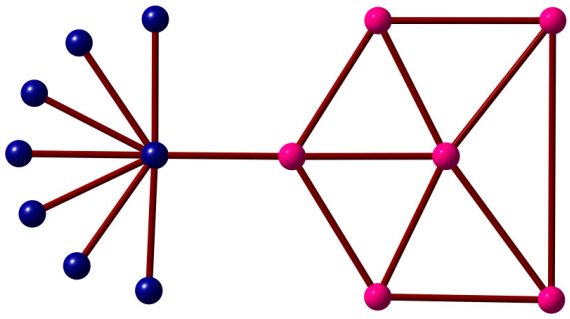


Figure 4: An example of G in which $Mo_t(G) \neq Mo_v(G) + Mo_e(G)$

The computational technique for the Mostar indices relies on the cut method which is in turn based on the Djoković-Winkler relation defined on the edge set of a graph G as follows. Two edges $e_1 = c_1d_1$ and $e_2 = c_2d_2$ are in relation Θ if $d_G(c_1, c_2) + d_G(d_1, d_2) \neq d_G(c_1, d_2) + d_G(c_2, d_1)$. The relation Θ is reflexive and symmetric, but not transitive in general whereas the transitive closure Θ^* forms an equivalence relation thereby enabling the Θ^*-partition of the edge set $E(G)$ as $E_1, \ldots, E_p$. These classes split each of the graphs $G - E_i$ into two or more smaller components. The quotient graph G/E_i is defined as a graph in which the vertices are the connected components of $G - E_i$, and two components A_1 and A_2 are linked by an edge if there exists an edge $xy \in E_i$ such that $x \in A_1$ and $y \in A_2$. The computational technique for the Mostar indices was developed in [5] as follows. Let G be a molecular graph that admits a Θ^*-partition $\mathscr{E}(G) = \{E_1, \ldots, E_p\}$. If $Mo \in \{Mo_v, Mo_e\}$, then

$$Mo(G) = \sum_{i=1}^{p} Mo(G/E_i, (w_v^i, s_v^i), s_e^i),$$

where

(i) $w_v^i : V(G/E_i) \to \mathbb{R}_0^+$, $w_v^i(X) = \sum_{x \in V(X)} w_v(x)$, $\forall\ X \in V(G/E_i)$,

(ii) $s_v^i : V(G/E_i) \to \mathbb{R}_0^+$, $s_v^i(X) = \sum_{xy \in E(X)} s_e(xy) + \sum_{x \in V(X)} s_v(x)$, $\forall\ X \in V(G/E_i)$,

(iii) $s_e^i : E(G/E_i) \to \mathbb{R}_0^+$, $s_e^i(XY) = \sum_{\substack{xy \in E_i \\ x \in V(X),\ y \in V(Y)}} s_e(xy), \forall\ XY \in E(G/E_i)$.

2 Corrected Results

The inappropriate mathematical construction of Θ-classes of SiO_2 nanosheet, i.e., failing to satisfy transitive property with respect to Djoković-Winkler relation and failing to locate suitable Θ^*-classes in the recent paper [1] are the causes of incorrect results in [1] as demonstrated here. Subsequently, we show the correct construction of Θ^*-classes. On the basis of that, we have obtained the correct Mostar indices by utilizing the concept of strength-weighted graphs.

To illustrate, consider the SiO_2 nanosheet of dimension $[2, 3]$ and its vertices a_1, a_2, a_3, b_1, b_2, b_3, c_1, c_2, and c_3 as shown in Figure 5.

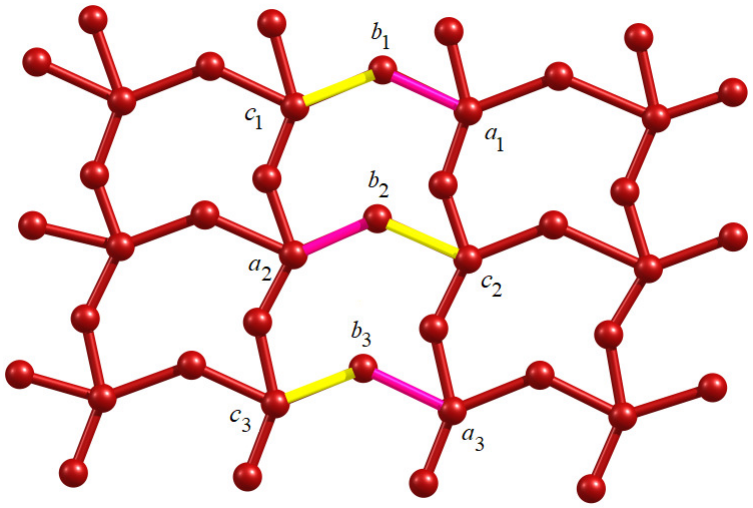


Figure 5: Construction of Θ^*-class in SiO_2 nanosheet

Let $D = \{a_1b_1, a_2b_2, a_3b_3\}$. Then it is claimed in [1] (see Figure 4 of Ref [1]) that the edges from D form a convex cut (alias a Θ-class), which is in fact false. First of all, the vertices b_1 and b_2 are members of opposite edges on the 8-cycle, and hence they need to lie in different parts of the asserted convex cut. But since the same holds for the pair b_1 and b_3 and for the pair b_2 and b_3, we get a contradiction. In the language of the relation Θ, we easily see that a_1b_1 is in relation Θ with a_2b_2, and that a_2b_2 is in relation Θ with a_3b_3. However a_1b_1 is not Θ related to a_3b_3. By the transitivity, the edges from D must lie in a common Θ^*-class. Let next $D' = \{b_1c_1, b_2c_2, b_3c_3\}$, see the yellow edges in Figure 5. As for D we infer that the edges from D' must also lie in a common Θ^*-class. Note now that b_1c_1 is Θ related with a_3b_3. Using the transitivity again we see that all the edges from $D \cup D'$ must lie in a common Θ^*-class. Finally, observe that no edge from $D \cup D'$ is Θ related with any edge outside this set. This fact can be most easily deduced by noticing that between an edge in $D \cup D'$ and an edge outside of this set, we can find a shortest path (in a Manhattan metric's style) with these two edges being the end edges of the path. For the latter argument we recall that no two edges of a shortest path are Θ related. Thus, since no edge from $D \cup D'$

is Θ related with any edge outside this set, we conclude that $D \cup D'$ is a Θ^*-class of the SiO_2 nanosheet of dimension $[2,3]$. By symmetry, it is clear from here as to which members are all the other Θ^*-classes. The arguments as explained above will be used throughout the section without detailed explanations.

Though the preceding graphic representation clearly shows the mathematical computational defects that happened in calculating the Mostar indices of SiO_2 nanosheets, we now present the numerical inaccuracies that occurred in Mostar analytic expressions. It was found in [1] that $Mo_v(\mathrm{SiO}_2[p,q]) = 2(3pq+4q+4p+3)\big((q+1)\big(2\lceil\frac{p}{2}\rceil - p+1\big) + (p+1)\big(2\lceil\frac{q}{2}\rceil - p+1\big)\big) - 2(q+1)(3q+4)\big(2\lceil\frac{p}{2}\rceil\big(\lceil\frac{p}{2}\rceil+1\big) - p(p+1)\big) - 2(p+1)(3p+4)\big(2\lceil\frac{q}{2}\rceil\big(\lceil\frac{q}{2}\rceil+1\big) - q(q+1)\big)$, and in particular, $Mo_v(\mathrm{SiO}_2[4,5]) = 6942$. However, independent computational methods [2] have confirmed that $Mo_v(\mathrm{SiO}_2[4,5]) = 5952$ is the correct value and our numerical result was obtained for $\mathrm{SiO}_2[4,5]$ upon substituting $p=4$, $q=5$ in our expression (1) of Theorem 1.

As previously discussed, a Θ^*-class of SiO_2 nanosheet or C_8 layer structure composed of all zig-zag bonds of specific row produces a quotient graph $K_{2,q+1}$, complete bipartite graph with vertex partition sets $\{X_1, X_2\}$ and $\{Y_i : 1 \le i \le q+1\}$ with weighted measures denoted by $w_v(X_1) = w_1$, $s_v(X_1) = s_1$, $w_v(X_2) = w_2$, $s_v(X_2) = s_2$, $w_v(Y_i) = 1$, $s_v(Y_i) = 0$ and $s_e(X_kY_i) = 1$ where $k = 1, 2$.

Theorem 1. *Let* $\mathrm{SiO}_2[p,q]$ *be an* SiO_2 *nanosheet of dimension* $[p,q]$.

1. $Mo_v(SiO_2[p,q]) = \frac{1}{2}(12p^2q^2 + 26pq^2 + 26p^2q + 23q^2 + 56pq + 23p^2 + 37p + 37q + (-1)^p(q^2+7q+6) + (-1)^q(p^2+7p+6) + 12)$

2. $Mo_e(SiO_2[p,q]) = 8p^2q^2 + 16pq^2 + 16p^2q + 11p^2 + 32pq + 11q^2 + 18p + 18q + (-1)^p(q^2+4q+3) + (-1)^q(p^2+4p+3) + 6$

Proof. For $1 \le i \le 2(q+1)$, let VP_i be an SiO_2 nanosheet peripheral vertical pendant bond. The quotient graph $\mathrm{SiO}_2[p,q]/VP_i$ is the complete bipartite graph $K_{1,1}$ with partite sets $\{A_i^p\}$ and $\{B_i^p\}$ with vertex weights $w_v^i(A_i^p) = 1$, $w_v^i(B_i^p) = 3pq+4(p+q)+4$, vertex strengths $s_v^i(A_i^p) = 0$, $s_v^i(B_i^p) = 4(pq+p+q+1)-1$, and edge strength $s_e^i(A_i^pB_i^p) = 1$. For $1 \le i \le p$, let VR_i be a Θ^*-class that contains all the vertical zig-zag bonds in the i^{th} row. In this class, the quotient graph is the complete bipartite graph $K_{2,q+1}$ with weighted measures $w_1 = (3q+4)i$, $s_1 = (q+1)(4i-1)$, $w_2 = (3q+4)(p+1-i)$ and $s_2 = (q+1)(4(p-i)+3)$. We consider the classes HP_i $(1 \le i \le 2(p+1))$ and HC_i $(1 \le i \le q)$ as analogous to vertical zig-zag type bonds and the graph theoretical quantities are obtained by swapping the values of p and q. If we take $Mo \in \{Mo_v, Mo_e\}$, and denote $\sum_{i=1}^{2(q+1)} Mo(\mathrm{SiO}_2[p,q]/VP_i) + \sum_{i=1}^{p} Mo(\mathrm{SiO}_2[p,q]/VR_i) = f(p,q)$, then $\sum_{i=1}^{2(p+1)} Mo(\mathrm{SiO}_2[p,q]/HP_i) + \sum_{i=1}^{q} Mo(\mathrm{SiO}_2[p,q]/HC_i) = f(q,p)$ and $Mo(\mathrm{SiO}_2[p,q]) = f(p,q) + f(q,p)$. □

Theorem 2. *Let* $C_8[p,q]$ *be a* C_8 *layer structure of dimension* $[p,q]$.

1. $Mo_v(C_8[p,q]) = \frac{1}{2}(12p^2q^2+10pq^2+10p^2q+3q^2+3p^2-5q-5p+(-1)^p(q^2+5q+4)+(-1)^q(p^2+5p+4)-8)$

2. $Mo_e(C_8[p,q]) = 8p^2q^2+6pq^2+6p^2q+p^2+q^2-3q-3p+(-1)^p(q^2+3q+2)+(-1)^q(p^2+3p+2)-4$

Proof. The proof technique is similar to $SiO_2[p,q]$ and we take VR_i $(1 \leq i \leq p)$ to represent the Θ^*-class that covers all the zig-zag vertical bonds in the i^{th} row of $C_8[p,q]$. The corresponding quotient graph is the complete bipartite graph $K_{2,q+1}$ with weighted measures $w_1 = q(3i-1)+(2i-1)$, $s_1 = 2i(2q+1)-2(q+1)$, $w_2 = 3q(p-i)+2(p+q-i)+1$ and $s_2 = (4q+2)(p-i)+2q$. Let HC_i $(1 \leq i \leq q)$ be an analogous Θ^*-class that covers all vertical zig-zag bonds and the graph theoretical measures are produced by exchanging p and q values. If we denote $\sum_{i=1}^{p} Mo(C_8[p,q]/VR_i) = g(p,q)$, then $\sum_{i=1}^{q} Mo(C_8[p,q]/HC_i) = g(q,p)$ and $Mo(C_8[p,q]) = g(p,q)+g(q,p)$ where $Mo \in \{Mo_v, Mo_e\}$. □

We close this section by pointing out the constructional inconsistency [1] for the melem chain due to hydrogen atoms and also numerous inaccuracies in the computation of Mostar indices, in particular, treating the cardinality of bond additive sets of horizontal and slanting bonds equally. The proper construction of a melem chain [6] can be done using the unit cell shown in Figure 3b. Finally, we would like to mention that $Mo_t(G) = Mo_v(G)+Mo_e(G)$ for both SiO_2 nanomaterials and melem nanostructures because $n_u(h|G) \geq n_v(h|G)$ and $m_u(h|G) \geq m_v(h|G)$ or $n_u(h|G) \leq n_v(h|G)$ and $m_u(h|G) \leq m_v(h|G)$ for every edge h in G.

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