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Pauli Repulsions Exist Only in the Eye of the Beholder

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Abstract: This paper presents a rebuttal to the preceding paper in this issue entitled "Hydrogen-Hydrogen Bonding in Planar Biphenyl, Predicted by Atoms-In-Molecules Theory, Does Not Exist". The arguments presented therein are based on an arbitrary partitioning of the energy into contributions from physically unrealizable states of the system. The response given here is presented in terms of the Feynman, Ehrenfest, and virial theorems of quantum mechanics and the observable properties of a system. A reader is thus free to choose between subjectivity or physics.

Keywords: atoms-in-molecules (AIM) theory · bonding theory · electron density

Introduction

Science is observation and experiment followed by appeal to theory and a return to experiment. This philosophy, in the manner recently described,[1] led to the development of the quantum theory of atoms in molecules (QTAIM).[2] I was asked to referee the preceding paper by Poater, Solà, and Bickelhaupt[3] that is based on a subjective model invoking "Pauli repulsions" and does so at the attempted expense of physics, by criticizing the physics of an open system, QTAIM. As someone who accepts quantum mechanics, I know that there are only two forces operative in field-free chemistry: the Ehrenfest force acting on the electrons and the Feynman force acting on the nuclei. The molecular virial theorem relates the virial of the Ehrenfest force to the kinetic energy of the electrons, the molecular virial including a contribution from the virial of the Feynman forces acting on the nuclei. *Thus through the Ehrenfest and Feynman theorems, one has the tools that are needed to describe the forces acting in a molecule and through the virial theorem, to relate these forces to the molecule's energy and its kinetic and potential contributions in the manner promulgated by Slater.*[4]

This statement of physics posses a dilemma with respect to the work of Poater, Solà, and Bickelhaupt: there are no "Pauli or exchange repulsions" that Poater, Solà, and Bickelhaupt claim to be present between the *ortho*-hydrogens in planar biphenyl, a statement in contradiction with the finding that these hydrogens are linked by a bond path.[5] [The phrase "exchange repulsion" is an oxymoron—exchange reduces the electron–electron (e–e) epulsion.] Their result is arrived at through the introduction of arbitrarily chosen non-physical reference states that violate all of the rules of physics, in particular the Pauli principle. This criticism is aptly summarized by Morokuma himself[6] whose energy decomposition analysis (EDA) analysis provides the basis to their approach: "There is no unique choice for the intermediate wave functions, and they do not correspond to reality (e.g., "not all" satisfy the Pauli principle!)." [Morokuma's exclamation mark] The non-physical aspects of the EDA schemes of Morokuma or Zielgler and Rauk[7](as used by Poater, Solà, and Bickelhaupt) and their use by Frenking et al.[8] have been recently reviewed.[9] There is no shortage of imagined reference states that one can invoke to discuss barriers, as exemplified by the use of NBOs that ascribes steric repulsions to hyperconjugation through the initial omission and later inclusion of selected sets of orbitals.[10,11] As stressed by Bickelhaupt and Baerends in a sister journal,[12] "one can use neither physics nor observation to decide between the competing explanations of "Pauli repulsions" or "hyperconjugative electron release" as the cause of the ethane barrier" So where is science in all of this? The barrier in ethane has a simple physical explanation:[13] In terms of overall energy contributions, the barrier *is not repulsive*: it arises because of a decrease in the magnitude of the electron–nuclear (e–n) attractions that exceeds the accompanying *decrease* in the e–e and nuclear–nuclear (n–n) repulsions. In terms of the physics of an open system, the energy increase is confined to the two carbon atoms, a consequence of the increase in the C−C bond length accompanying the rotation to the eclipsed conformer, a lengthening

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that decreases the attraction of each C nucleus for the density in the neighboring C basin. Nor does a rotation with a fixed C–C separation cause repulsion between the hydrogens, as previously demonstrated.[13] There is no mystery—just simple physics.

"Pauli repulsions" and the Feynman force

The electrostatic contributions to the energy as enshrined in the Hamiltonian, are indeed tempered by the requirements of the Pauli principle. These requirements are described neither by "resonance" nor by "Pauli repulsions", but are instead determined through the mechanism of electron exchange, the consequence of incorporating the requirement of antisymmetry into the wave function. Quantum-mechanical exchange, defined by the exchange operator, plays a unique and important role in chemistry. The spatial localization/delocalization of electrons for example, is determined by the corresponding properties of the exchange density.[14,15] It has been amply demonstrated how the physical consequences of exchange can be determined directly within QTAIM[9] rather than being disguised in nonphysical terms such as "resonance", "Pauli or exchange repulsions" and "covalency". We are interested in particular in the effect of the antisymmetry requirements (the requirement of orbital orthogonality) on the electron density distribution for the approach of closed-shell atoms. This is most simply illustrated using the He_2 system through the use of density difference maps $\Delta\rho$ obtained by subtracting the density of the overlapping atomic densities from the molecular density for each internuclear separation.[9,16] The resulting $\Delta\rho$ provides a precise description of the "Pauli repulsions" used in EDA: the effect of imposing orthogonality on the orbitals defining the density of the overlapped free atoms.[17] The form of $\Delta\rho$ is exceedingly simple:[18] it removes density from the region of orbital overlap and accumulates it in the nonbonded regions, the Berlin binding and antibinding regions,[19] respectively, just the opposite of the $\Delta\rho$ maps obtained for the approach of two H atoms. This change in density results in electrostatic forces of repulsion acting on the nuclei. Thus the effect of antisymmetrization of the wave function is to remove density from the region of overlap of the occupied orbitals and to create an *electrostatic* force of repulsion on the nuclei. The "Pauli force" is in fact the Feynman[20] electrostatic repulsive force acting on the nuclei. There are no Feynman forces acting on the nuclei in an equilibrium geometry and for separations greater than the equilibrium separation the forces are attractive. Thus the antisymmetry requirement leads to repulsions on the nuclei—those required by the imposition of the Pauli principle—only for separations less than the equilibrium separations. *The only net repulsive force operative in a molecular system is the Feynman electrostatic force exerted on the nuclei.*

Anyone wishing to counter this statement of physics should perform the following calculation. Push any two atoms together—with or without charge transfer—and monitor the change in the total energy E and the change in just the electronic energy H_e which equals the total energy E minus the n–n energy of repulsion.[21] As R is decreased from R_e, E increases but H_e decreases monotonically to the united atom (UA) limit—even for He_2. The kinetic energy T, as required by the virial theorem, attains a limiting value equal to the negative of the energy of the UA. One might have expected H_e to shown some "bumps" as closed inner-shells come into contact—"closed-shell repulsions"—but this does not happen. Instead the e–n attractive potential overwhelms the increasing kinetic energy and the e–e repulsions and the UA energy is approached without any suggestion of intervening repulsions. Since E and H_e differ only by the n–n repulsion, the repulsion upon close approach of two atoms is a result of the overriding increase in the nuclear–nuclear repulsive energy. *Thus, according to physics, when repulsions do exist between atoms they are a consequence of the nuclear–nuclear repulsions dominating the total energy.* The sole repulsive contribution to the Ehrenfest force, the equal and opposite force that one atom exerts on the basin of its bonded neighbor, is from the e–e interaction. Thus the Ehrenfest force parallels the behavior of H_e, becoming attractive for separations in excess of R_e and becoming increasingly so, as the UA limit is approached.

The above is not the picture of repulsion between atoms that one obtains using EDA. The EDA definition of "Pauli repulsion" that Poater, Solà, and Bickelhaupt state "is responsible for any steric repulsion" is equated to the energy change that arises by imposing antisymmetry on the simple product wave function of arbitrarily chosen initial fragments that are prepared in the geometries they possess in the product molecule, in effect correcting for the improper overlap obtained by the superposition of the fragment densities. Thus one obtains Pauli repulsions by first violating the Pauli principle and then imposing it! Since neither the product state nor its antisymmetrized form satisfy quantum mechanics, it is not possible to apply the virial or the Feynman force theorem to determine the source of the increase in energy. The imposition of antisymmetry will cause changes in the density that will result in forces on the nuclei (the density is "relaxed" to its force-free product form consistent with the pre-assigned geometries only in the final step of EDA). Thus even accepting the arbitrary steps leading up to this stage, one cannot relate the energy increase to the presence or absence of Feynman forces of repulsion acting on the nuclei, the physical manifestation of the Pauli principle.

After presenting the arguments rationalizing EDA, Poater, Solà, and Bickelhaupt arrive at—what is to them—the contradictory finding that the Pauli repulsion *decreases* when the twisted equilibrium structure of biphenyl assumes the planar geometry, a result that favors the QTAIM finding of bonding between the *ortho*-hydrogens, as evidenced by the presence of a bond path.[5]

Truly, one of the advantages of the EDA approach is that one is free to define new reference states as needed to obtain a desired result. Poater, Solà, and Bickelhaupt simply replace motion on the minimum energy path on the potential energy surface (PES) predicted by quantum mechanics with motions far removed from the path that correspond to keeping all geometrical parameters fixed other than the angle of rotation. Such paths would not be sampled in any trajectory study and are physically improbable. The result of this added arbitrary step is that the Pauli repulsions are now a minimum for the twisted geometry. Poater, Solà, and Bickelhaupt confuse the analysis of the properties of the minimum energy states of a system with how the system might achieve these states. Confining their analysis to the physical states under question, where the densities and geometries are relaxed to their physically correct descriptions, leads to the result that the *ortho*-hydrogens in the planar geometry experience a lesser "Pauli repulsion" than when in the twisted geometry. Of course, this conclusion carries no more physical weight than the opposing view they prefer.

Applying the quantum mechanics of an open system

We begin the discussion of the underlying physics with a critique of their section entitled "Origin of H–H stabilization in AIM theory" where the authors display a lack of knowledge of the physics of an open system and in particular, of the virial theorem. We first note that thanks to Schwinger,[22] the physics of an open system is now *the* general statement of QM, the physics of a closed isolated system being a special limiting case of the general equation of motion for any observable $\hat{G}$ given in Equation (1) .[2,23]

$$N\int_{\Omega} d\mathbf{r}\int dr'\partial\{\Psi^{*}\hat{G}(\mathbf{r})\Psi+cc\}/\partial t= \\ \{(i/\hbar)\langle\Psi|[\hat{H},\hat{G}(\mathbf{r})]|\Psi\rangle_{\Omega}+cc\}-\oint d\mathbf{S}(\mathbf{r}_s;\Omega)\cdot\{\mathbf{J}_G(\mathbf{r}_s)+cc\} \tag{1}$$

Equation (1) applies to any spatial region satisfying the QM boundary condition of exhibiting a zero-flux in $\nabla\rho(\mathbf{r})$. The theorems of "ordinary" QM result from the vanishing of the surface term.

Setting $\hat{G}=-i\hbar\nabla$, an electronic momentum operator yields the Ehrenfest force theorem—the force acting on the electron density—the force acting on an *atom* in a molecule. Setting $\hat{G}=-i\hbar\nabla_{\alpha}$, the momentum operator for nucleus α yields the Feynman force theorem and the force acting on the *nucleus* of the atom. There is no operator corresponding to the "Pauli momentum" and the corresponding force does not exist.

Setting $\hat{G}=\mathbf{r}\cdot\mathbf{p}$ yields the generalized virial theorem and, for a molecule in electrostatic equilibrium in a stationary state, one obtains the Poater, Solà, and Bickelhaupt Equation (6) for E(A), the energy of atom A in a molecule. All open system properties are additive and, since they are derived from physics, recover all measurable properties. The authors' statement that "While mathematically well defined, the physical status of this quantity E(A) is not so clear." cannot be justified. First, it is not only mathematically well defined, it is derived from the most fundamental statement of *physics* presently at our disposal—the principle of stationary action.[22] Second, while realizing that one is addressing people who use models that cannot be tested against observation—EDA makes no physical predictions—this failing does not apply to QTAIM. In all cases where atomic or group properties are found to be experimentally additive; heats of formation—including measured strain and "resonance" energies; magnetic susceptibilities, including aromatic exaltation; polarizabilities, volumes etc, the group contributions determined by the physics of an open system agree with the experimental values.[24–26] What other test is there of a theory? What more can one possibly do to establish the "physical status" of E(A) or any other QTAIM property? In what respect does QTAIM fail to meet all scientific measures of a proper theory: it is based upon observation, derived from fundamental physics and recovers what can be measured?[27] Poater, Solà, and Bickelhaupt failed to respond to these questions, choosing to ignore the single test one has of a scientific theory—prediction. It is this philosophy that underlies Hans Bethe's view of science: "its great advantage is you can prove something is true or something is false", a statement he further paraphrased as "In science, you know you know."[28]

Now to their misunderstanding of the virial theorem and the role of the kinetic energy T. The molecular virial theorem[29] is surely the most abused of all theorems in quantum chemistry, with the Feynman electrostatic theorem[20] running a close second.[30–32] Slater regarded these as two of the most powerful theorems applicable to molecules and solids.[33] It is a common fallacy to associate an increase in T with the presence of a repulsion, as done by the present authors. The virial theorem states that $-2T$ equals the virial of the Ehrenfest forces acting on the electrons—on the electron density. The role of this force in bonding has recently been described and discussed in detail.[34] The virial of the Ehrenfest force equals the total potential energy of the molecule, the e–n attractive potential energy and the e–e and n–n repulsive contributions together with the virial of the external forces acting on the nuclei. The external forces are the Feynman forces required to hold the nuclei in a non-equilibrium geometry.[29] The relevant expression relating T and E for a diatomic (to keep the example as simple as possible) is $T=-E+RF(R)$ where $F(R)$ is the Feynman force $F(R)=-dE/dR$: attractive for $F(R)<0$ and repulsive for $F(R)>0$. One may rewrite this expression for the changes in T and E between any two states that have vanishing Feynman forces (the equilibrium and planar transition state in biphenyl, for example), as $\Delta T=-\Delta E+RF(R)$. For $R<R_e$, $\Delta T>-\Delta E$, the Feynman forces are repulsive and the contribution of the nuclear virial $RF(R)$ to the potential energy is positive and destabilizing. For $R>R_e$, $\Delta T<-\Delta E$, the forces are attractive and the nuclear virial is stabilizing. *No Feynman force* acts on an atom for a change in energy for which $\Delta T=-\Delta E$, the H atoms in H–H bonding being a case in point.[5]

The rotation of one phenyl group with respect to the other about the equilibrium value of the angle $\varphi\sim46°$, results in the formation of a singularity in the density between each pair of *ortho*-H atoms when φ is decreased to ~25°. With a further decrease in φ, each singularity bifurcates into a bond and ring critical point, an interatomic surface appears between the H atoms and their nuclei are linked by a line of maximum density—a bond path—that is strengthened to its limiting value at $\varphi = 0°$. Thus the atoms are bonded to one another and, *as is always the case on the formation of a bond path, their energy decreases.* Thus, relative to the equilibrium geometry, $\Delta E(\mathrm{H}) < 0$ in attaining the transition state geometry where the Feynman forces vanish. The change in the electronic kinetic energy $\Delta T(\mathrm{H})$, necessarily increases so that $\Delta T(\mathrm{H}) = -\Delta E(\mathrm{H})$ and the atomic volumes necessarily decrease, a consequence of the bonding drawing the atoms together.

Poater, Solà, and Bickelhaupt claim that since this process occurs without a significant transfer of charge, the atomic stabilization of the *ortho*-H atoms during this conformational change is due entirely to the reduction of their volumes—a result of the steric congestion between them—that causes their kinetic energies to increase. Thus the authors relate the decrease in energy of the *ortho*-H atoms not to the formation of a bond path linking them, but to the reduction in their volumes that raises their kinetic energy, thus reducing their total energy. In effect, Poater, Solà, and Bickelhaupt argue that stabilization of the *ortho*-H atoms is due to steric repulsion! Steric repulsion is not defined within physics and cannot be invoked in a discussion based on the virial theorem. $\Delta T(\mathrm{H})$ can be equated to $-\Delta E(\mathrm{H})$ only in the absence of net forces.

To further make clear the unphysical basis of this result, one first notes that the bonding process between two *ortho*-H atoms described above applies equally to the formation of the hydrogen molecule. There is no transfer of charge in the formation of a bond path between a pair of identical atoms and their volumes necessarily decrease, all as found for the *ortho*-H atoms. *The physics of bonding and the formation of a bond path between two hydrogen atoms in H_2 is indistinguishable from the bonding and the formation of a bond path between the ortho-H atoms in biphenyl.*[5] This is the physical basis underlying the statement that the presence of a bond path is a universal indicator of bonding.[35] In both cases—in all cases of bonding, *as signified by the formation of the bond path*, electron density is accumulated in the internuclear region and the initially *attractive* Feynman forces vanish as the separation decreases to the equilibrium value. The potential energy is decreased (i.e., becomes more stabilizing) and the energies of the atoms decrease because of the increase in the electron–nuclear attraction, the only attractive interaction in chemistry.[36] Thus H–H bonding and the bonding in H_2 differ not in kind—the physics of their bonding mechanisms being identical—they differ only in degree, one interaction being ten times larger than the other.

The arguments that are advanced to counter the results demanded by the virial theorem are manifold, as exemplified by the one put forth here concerning the 'steric congestion resulting from the reduction in the volume of the *ortho*-H atoms'. This argument makes no physical sense. All bonding results in a reduction in the volumes of the interacting atoms. Thus the volume of a hydrogen atom decreases by 66 % on forming H_2 compared to 5 % upon H–H bonding in biphenyl,[5] a result that according to Poater, Solà, and Bickelhaupt, would imply that the larger bonding energy in H_2 compared to H–H bonding is because of a greater steric congestion in H_2.

The quantum definition of the pressure acting on an atom is determined by its surface virial, a term proportional to the pressure–volume product.[37] Every bound atom is under pressure, the equilibrium pressure being determined by the condition that $T(\mathrm{A}) = -E(\mathrm{A})$. Atoms under pressure resulting from the application of an external constraining force that holds the system in an non-equilibrium geometry, must according to the virial theorem, exhibit a kinetic energy $T(\mathrm{A})$ in excess of $-E(\mathrm{A})$, the disparity increasing with increasing pressure. *Thus atoms under external pressure possess excess kinetic energies as a consequence of repulsive Feynman forces and the force responsible for the repulsion between atoms on close-approach is the nuclear-nuclear force of repulsion.* The virial theorem provides a simple litmus test for the presence of a repulsive force, denoted by $T(\mathrm{A}) > -E(\mathrm{A})$, or of an attractive force, denoted by $T(\mathrm{A}) < -E(\mathrm{A})$, acting on the nucleus of atom A in a molecule. For the *ortho*-H atoms in planar biphenyl, one finds $T(\mathrm{H}) = -E(\mathrm{H})$, implying the absence of any Feynman force.

The recent study of the Ehrenfest force[34] that one atom exerts on its bonded neighbor, enables one to extend the definition of bonding between atoms denoted by a bond path: the presence of a line of maximum density linking a pair of nuclei in an equilibrium geometry of a bound state or one lying within the attractive region of a potential well, implies not only the *absence* of repulsive Feynman forces on the nuclei but also the presence of an *attractive* Ehrenfest force acting across the interatomic surface drawing the two atoms together. To this one must add the observed structural homeomorphism between the electron density and the virial field.[38] Thus every bond path is mirrored by a virial path linking the same nuclei along which the potential energy density is maximally stabilizing. The associated virial graph delineates the lowering in energy associated with the formation of the structure defined by the molecular graph. These observations hold in all cases—intramolecular or intermolecular interactions.[39]

Molecular graphs have been shown to recover all chemical structures that were previously inferred from classical models of bonding in conjunction with observed physical and chemical properties. There is always agreement between an accepted classical structure and the molecular graph, even in the case of electron deficient molecules such as the boranes which, as a result of spectroscopic observations, required the extension of the classical model to include bridging hydrogens and two-electron three-center bonding.[40] In addition, the dynamics of the gradient vector field caused by displacements of the nuclei, defines all possible structures and, through the theory of structural stability, the mechanisms of structural change.[2,41] Poater, Solà, and Bickelhaupt are challenged to demonstrate a weakness or failure of physics in accepting the universality of a bond path as the necessary and sufficient condition for the definition of bonding between atoms.[35] Their statement that this "is an unproven premise" is at odds with both observation and physics.

Discussion and Conclusion

Apparently, Poater, Solà, and Bickelhaupt and others that they refer to such as Cioslowski[42] and Haaland,[43] have the ability to distinguish between interactions that are indistinguishable by physics alone. They simply "know" that in some cases a bond path implies bonding, while in others it implies the existence of repulsive forces, even though no net forces are present. Cioslowski and Mixon state that the term bond path should be reserved for "strong bonds", they apparently deciding where the cut-off occurs between strong and not so strong. In another example, Cioslowski et al.[44] state that the interactions between the chlorine atoms in a perhalogenated cyclohexane ring are "clearly repulsive" (even in an equilibrium geometry) and their linking by a bond path is a failure of QTAIM. In reality, as previously discussed,[35] the same interactions, identical in all details, are found for the intermolecular bond paths linking the chlorine atoms in solid Cl_2, their presence and directionality being readily rationalized in terms of the topology of the Laplacian of the density, thereby accounting for the layered structure of this solid.[45] If the Cl−Cl "nonbonded" interactions were indeed repulsive, solid chlorine could not exist! Haaland et al.[43] question the presence of bond paths found to link the He and ^{t}C atoms in the He@adamantane inclusion complex, interactions that they describe as "strongly antibonding". The QTAIM analysis of such inclusion complexes indicates that, as anticipated for an equilibrium structure, there are no Feynman forces exerted on the nuclei and that in addition, the Ehrenfest force acting on the He|C surface is attractive, drawing the two atoms together. Thus the He atom is stabilized with respect to the reactants, $\Delta E(\mathrm{He}) < 0$ and $\Delta T(\mathrm{He}) = -\Delta E(\mathrm{He})$. The endothermic energy change in forming the *stable* complex is absorbed in its entirety by a relaxation of the adamantage cage. The stabilization of the He atom in the adamantine cage is entirely analogous to the stabilization of a transition metal atom in the interior of its carbonyl complex.[9] I challenge Poater, Solà, and Bickelhaupt to provide a physical definition of the "strongly antibonding He···^{t}C interactions" claimed to be present by them and by Haaland et al.

Matta et al.[5] point out that H−H bonding is ubiquitous, their stabilization energies contributing to the sublimation energies of hydrocarbons. If the H−H bond paths that are topologically inescapable in solid methane represent "nonbonded, repulsive" interactions in the manner described by Poater, Solà, and Bickelhaupt for the physically indistinguishable H−H bonding in biphenyl, then what interactions, pray tell, account for the existence of solid methane? Identical H−H bonding is found between the hydrogen atoms bonded to the C1–C4 atoms in phenanthrene and other angular polybenzenoids, but are not commented on by Poater, Solà, and Bickelhaupt. Their presence accounts for the increased stabilities of the angular phenanthrene and chrysene over their respective linear isomers, hardly a result that can be ascribed to "nonbonded repulsive interactions".

The PES connecting the twisted and planar conformers of biphenyl is well-studied experimentally.[46] It is not related in any way whatsoever with the energy changes associated with the formation of biphenyl from two phenyl radicals through a series of imagined intermediate states, the model used by Poater, Solà, and Bickelhaupt in EDA, much less with their model of tetra-radical with a quintet ground state. QTAIM, by offering the possibility of answering all questions at the atomic level through physics, removes the necessity of invoking states, real or imagined, to achieve an understanding. One need only recall that the electron density obtained in a variational calculation is the distribution that minimizes the energy for any geometry and thus the presence of bond paths represent spatial accumulations of the density that lower the energy of the system. Their properties provide a physical classification of the interactions in terms of an observed property of a system, free of any reference states, as opposed to Poater, Solà, and Bickelhaupt who do not observe reality, but view it through glasses that distort it to whatever they wish to perceive.

Their concluding statement: "All together, there is an increasing body of evidence that the physical interpretation of AIM concepts, such as bond paths and atomic stabilization energies, is unclear" is at variance with the demonstrated agreement with and recovery of experiment by QTAIM. Their statement is based upon neither physics nor observation. Cioslowski and Haaland, along with the present authors must be contacted so as to inquire whether a bond path observed in any particular case denotes "bonding" or "repulsion", since this question has no meaning within the realm of physics. QTAIM requires only knowledge of the density and of quantum mechanics and no outside assistance is required for either its derivation or application. All conclusions are made by appeal only to physics.[47]

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[47] Note added in proof (2. 2. 2006): In a final risposte, I would just like to mention that in their reply to my comments Poater, Solà, and Bickelhaupt (J. Poater, M. Solà, F. M. Bickelhaupt, *Chem. Eur. J.* **2006**, *12*, DOI: 10.1002/chem.200600057) use the unphysical models that violate quantum mechanics and they are thus prevented from predicting experimentally measurable properties. QTAIM is quantum mechanics obtained from Schwinger's principle, a relativistically invariant theory, and thus predicts all measurable properties.

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