Flexible C_{6}BN Monolayers As Promising Anode Materials for High-Performance K-Ion Batteries

Pan Xiang, Sitansh Sharma, Zhiming M. Wang, Jiang Wu,* and Udo Schwingenschlögl*

ABSTRACT: K-ion batteries attract extensive attention and research efforts because of the high energy density, low cost, and high abundance of K. Although they are considered suitable alternatives to Li-ion batteries, the absence of high-performance electrode materials is a major obstacle to implementation. On the basis of density functional theory, we systematically study the feasibility of a recently synthesized C_{6}BN monolayer as anode material for K-ion batteries. The specific capacity is calculated to be 553 mAh/g (K_{2}C_{6}BN), i.e., about twice that of graphite. The C_{6}BN monolayer is characterized by high strength (in-plane stiffness of 309 N/m), excellent flexibility (bending strength of 1.30 eV), low output voltage (average open circuit voltage of 0.16 V), and excellent rate performance (diffusion barrier of 0.09 eV). We also propose two new C_{6}BN monolayers. One has a slightly higher total energy (0.10 eV) than the synthesized C_{6}BN monolayer, exhibiting enhanced electronic properties and affinity to K. The other is even energetically favorable due to B−N bonding. All three C_{6}BN monolayers show good dynamical, thermal, and mechanical stabilities. We demonstrate excellent cyclability and improved conductivity by K adsorption, suggesting great potential in flexible energy-storage devices.

KEYWORDS: energy storage, K-ion battery, flexible anode, C_{6}BN monolayer, first-principles calculation

INTRODUCTION

The limited reserves of traditional energy sources and the environmental issues caused by them make the development of clean sustainable energy sources an urgent task. However, these sources, such as solar energy and wind energy, are greatly affected by environmental and weather conditions, resulting in fluctuating output. Therefore, large scale energy storage systems are required that combine safety, stability, and low cost. In addition, emerging electric vehicles and wearable electronics need high performance (high capacity, fast charging) batteries as power source. Regrettably, the current commercial Li-ion batteries are not able to fulfill these demands because of a shortage of Li sources and their uneven global distribution. On the other hand, K-ion batteries can rely on abundant K sources. In combination with fast ion transport in the electrolyte this makes them to promising alternatives for large scale energy storage systems and electric vehicles. In this context, it is essential to develop for K-ion batteries suitable low cost and high performance electrode materials, as they determine their electrochemical properties.

Interestingly, graphite, the most mature anode material applied in Li-ion batteries, is not suitable for Na-ion batteries but can be used to store K. However, because of the larger atomic radius of K as compared to Li, only one K atom can be stored per eight C atoms, corresponding to a specific capacity of 279 mAh/g. On the basis of first-principles calculations, the binding energy of a single K atom on graphene was found to be 1.05 eV, which is only slightly larger than the cohesive energy of K (0.93 eV), indicating potential risk of dendrite formation. While the electrochemical performance of C-only anode materials is unsatisfactory for K-ion batteries, improvement is found for two-dimensional C_{3}B. Two-dimensional C_{3}N provides a high specific capacity of 1072 mAh/g, however, only through multilayer adsorption. For Li-ion batteries the electrochemical performance of ternary B−C−N anode materials (borocarbonitrides) was studied systematically, proposing that C-rich B_{0.13}C_{0.73}N_{0.12} Provides the highest surface area and specific capacity. Recently, a C-rich borocarbonitride monolayer, C_{6}BN, could be synthesized using a low cost two-step borylation reaction. The material combines valley-selective circular dichroism with high carrier mobility, consistent with the conclusion that higher C content in borocarbonitrides improves the conductivity. This development together with the low mass density and...
possibility of low-cost fabrication motivates us to explore C$_6$BN monolayers as anode materials for K-ion batteries.

We determine the basic properties and electrochemical performance of the synthesized C$_6$BN monolayer and put forward two other C$_6$BN monolayers based on first-principles calculations. For each of the three C$_6$BN monolayers we first optimize the structure and examine the stability. Then, the band structure, density of states, Young’s modulus, Poisson’s ratio, and out-of-plane bending stiffness are studied to obtain insights into the electronic structure, in-plane strength, and flexibility. We also evaluate the adsorption and diffusion of K on the C$_6$BN monolayers. The specific capacity and open

Figure 1. C$_6$BN monolayers: (a–c) Top and side views of the optimized structure with Brillouin zone and electron localization function. (d–f) Phonon dispersion relation. (g–i) Total potential energy during the ab initio molecular dynamics simulation with final structure and radial distribution functions.
circuit voltage (OCV) are calculated by obtaining the energetically favorable structures of potassiated C$_6$BN monolayers. Finally, the effect of K adsorption in the conductivity of the C$_6$BN monolayers is investigated.

**COMPUTATIONAL DETAILS**

First-principles calculations are performed by the DMol$^3$ program using a double-numerical polarized basis, the all electron relativistic method, and the Perdew–Burke–Ernzerhof generalized gradient approximation of the exchange-correlation functional. The Grimme dispersion correction is adopted to describe the long-range van der Waals interaction.$^{26}$ The convergence thresholds of the energy, maximum force, and displacement in the structure optimization are set to $1.0 \times 10^{-6}$ Ha, 0.001 Ha/Å, and 0.002 Å, respectively. Convergence tests (Figure S1) show that a Monkhorst–Pack 7 $\times$ 7 $\times$ 1 k-mesh for sampling the Brillouin zone provides reliable results. A small smearing of $5 \times 10^{-4}$ Ha and a large global orbital cutoff of 5.6

### Table 1. Structural Details, Relative Energy, and Material Properties

<table>
<thead>
<tr>
<th></th>
<th>lattice constant (Å)</th>
<th>C−B bond length (Å)</th>
<th>C−C bond length (Å)</th>
<th>C−N bond length (Å)</th>
<th>B−N bond length (Å)</th>
<th>relative energy (eV)</th>
<th>band gap (eV)</th>
<th>bending stiffness (eV)</th>
<th>Young’s modulus (N/m)</th>
<th>Poisson’s ratio</th>
</tr>
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<tbody>
<tr>
<td>C$_6$BN-I</td>
<td>4.982</td>
<td>1.473</td>
<td>1.412</td>
<td>1.456</td>
<td>0</td>
<td>1.28</td>
<td>1.30</td>
<td>310</td>
<td>311</td>
<td>0.176</td>
</tr>
<tr>
<td>C$_6$BN-II</td>
<td>4.983</td>
<td>1.477</td>
<td>1.430</td>
<td>1.421</td>
<td>0.10</td>
<td>0.13</td>
<td>1.36</td>
<td>317</td>
<td>312</td>
<td>0.175</td>
</tr>
<tr>
<td>C$_6$BN-III</td>
<td>4.975</td>
<td>1.485</td>
<td>1.428</td>
<td>1.411</td>
<td>1.455</td>
<td>−1.10</td>
<td>1.16</td>
<td>1.38</td>
<td>314</td>
<td>317</td>
</tr>
</tbody>
</table>

Figure 2. C$_6$BN monolayers: (a–c) Band structure and partial densities of states. (d) Armchair and zigzag directions. (e, f) Young’s modulus and Poisson’s ratio. (g–i) Energy per formula unit for C$_6$BN-I, C$_6$BN-II, and C$_6$BN-III nanotubes of different radius with insets showing the typical structure.
Å are employed in all calculations. To avoid artificial interaction between periodic images in the out-of-plane direction, a large vacuum thickness of 25 Å is used. To evaluate the thermal stability of the C\textsubscript{6}BN monolayers, we use ab initio molecular dynamics simulations at 300 and 1200 K (NVT ensemble) for 10 ps with a time step of 1 fs. Still adopting the Perdew–Burke–Ernzerhof and Grimme schemes, the dynamic stability is investigated by calculating the phonon spectrum by the Phonopy\textsuperscript{27} and VASP\textsuperscript{28} (projector augmented-wave potentials, 1 × 10\textsuperscript{-6} eV energy convergence threshold, Monkhorst–Pack 12 × 12 × 1 k-mesh) programs, and charge densities and electron localization functions are obtained by means of the CASTEP\textsuperscript{29} program (norm-conserving pseudopotentials, 5 × 10\textsuperscript{-7} eV/atom energy convergence threshold, Monkhorst–Pack 7 × 7 × 1 k-mesh).

\section*{RESULTS AND DISCUSSION}

\textbf{Structure, Stability, and Material Properties.} The synthesized C\textsubscript{6}BN monolayer has a hexagonal unit cell with space group P\textsuperscript{6}3m2 and point group D\textsubscript{6h} containing pure and B–N para-doped C rings, as shown in Figure 1a. We obtain a lattice constant of 4.982 Å and equilibrium C–C, C–B, and C–N bond lengths of 1.412, 1.473, and 1.456 Å, respectively, in agreement with previously reported results.\textsuperscript{21} Because of the bond energy order B–N (4.00 eV) > C–C (3.71 eV) > N–C (2.83 eV) > B–C (2.59 eV) > B–B (2.32 eV) > N–N (2.11 eV) in borocarbonitrides,\textsuperscript{30} B–N bonds are most favorable. However, as shown in Figure 1a, there exists no B–N bond in the synthesized C\textsubscript{6}BN monolayer (named C\textsubscript{6}BN-I in the following), probably because the synthesis is based on pyrolysis of specific precursors. By adjusting the sites of the B and N atoms in the hexagonal C network, we obtain two new monolayers, named C\textsubscript{6}BN-II and C\textsubscript{6}BN-III. Unlike C\textsubscript{6}BN-I, the unit and primitive cells of C\textsubscript{6}BN-II and C\textsubscript{6}BN-III are different because of reduced symmetry, the unit cell being orthogonal (Figure S2), and the primitive cell being almost hexagonal (angle very close to 120°; Figure 1b, c). To enable better comparison with C\textsubscript{6}BN-I, we used the primitive cells in further study. As shown in Figure 1b, c, C\textsubscript{6}BN-II (B–N meta-doped) and C\textsubscript{6}BN-III (B–N ortho-doped) stay perfectly planar. According to Table 1, the lattice constants and bond lengths of the C\textsubscript{6}BN monolayers are similar due to the identical elemental compositions and similarity of the crystal structures. Expectedly, introduction of strong B–N bonds in C\textsubscript{6}BN-III lowers the total energy by 1.10 eV per formula unit with respect to synthesized C\textsubscript{6}BN-I. The total energy of C\textsubscript{6}BN-II turns out to be only 0.10 eV higher than that of synthesized C\textsubscript{6}BN-I. Therefore, synthesis of C\textsubscript{6}BN-II and C\textsubscript{6}BN-III should be possible by the same method employed successfully in the case of C\textsubscript{6}BN-I. The insets in Figure 1a–c show the electron localization function for the C\textsubscript{6}BN monolayers to analyze the electron distribution and bonding features. Because of the comparable electronegativities of B, C, and N, high values (blue) between atoms indicate a covalent bond character as in the case of graphene.\textsuperscript{31}

To examine the dynamical stability of the C\textsubscript{6}BN monolayers, we study the phonon spectra. The absence of imaginary frequencies in the entire first Brillouin zone demonstrates dynamical stability, as shown in Figure 1d–f. The maximal frequencies of 1616, 1599, and 1591 cm\textsuperscript{-1} obtained for C\textsubscript{6}BN-I, C\textsubscript{6}BN-II, and C\textsubscript{6}BN-III, respectively, are comparable to those of C\textsubscript{3}N (1638 cm\textsuperscript{-1})\textsuperscript{32} and C\textsubscript{6}B (1510 cm\textsuperscript{-1})\textsuperscript{32} and indicate strong bonding. Ab initio molecular dynamics simulations are executed for each C\textsubscript{6}BN monolayer using a 3 × 3 supercell. As shown in Figure 1g–i, the fluctuations of the total energy are of the order of 0.01 eV at 300 K. The C\textsubscript{6}BN monolayers maintain their structure without relevant distortions, which is confirmed by peaks in the radial distribution functions at the equilibrium lengths of the C–B, C–C, and C–N bonds (insets of Figure 1g–i). Similar results are observed up to 1200 K (Figure S3), indicating excellent thermal stability to endure elevated temperatures during device operation. The mechanical stability of the C\textsubscript{6}BN monolayers is examined by determining the linear elastic constants, C\textsubscript{ij}, by fitting the energy of the orthogonal unit cell under armchair axial (\(\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \epsilon \\ 0 & \epsilon & 0 \end{pmatrix}\)), hydrostatic planar (\(\begin{pmatrix} \epsilon & 0 & 0 \\ 0 & \epsilon & 0 \\ 0 & 0 & \epsilon \end{pmatrix}\)), zigzag axial (\(\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \epsilon \\ \epsilon & 0 & 0 \end{pmatrix}\)), and shear (\(\begin{pmatrix} 0 & \epsilon & 0 \\ \epsilon & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\)) deformations for external strain \(\epsilon\) from −2% to 2% (steps of 0.5%). We obtain for C\textsubscript{6}BN-I, C\textsubscript{6}BN-II, and C\textsubscript{6}BN-III values of 320, 56, 321, and 131 N/m for C\textsubscript{6}BN-I; 327, 56, 322, and 132 N/m for C\textsubscript{6}BN-II; and 325, 59, 328, and 132 N/m for C\textsubscript{6}BN-III; i.e., in each case the Born criteria (C\textsubscript{11} > 0, C\textsubscript{22} > 0, C\textsubscript{11}C\textsubscript{22} − C\textsubscript{12} > 0, C\textsubscript{44} > 0)\textsuperscript{33} imply mechanical stability.

Having confirmed the structural stability of the C\textsubscript{6}BN monolayers, the band structure and partial densities of states are addressed in Figure 2a–c to examine the electronic properties. C\textsubscript{6}BN-I and C\textsubscript{6}BN-III show similar band structures with both the valence band maximum and conduction band minimum at the K point (band gaps of 1.28 and 1.16 eV, respectively). The partial densities of states indicate that the valence band edge is mainly due to the C and N atoms, whereas the conduction band edge is mainly due to the B and C atoms. C\textsubscript{6}BN-II is characterized by a very small direct band gap of only 0.13 eV at the K point with the bands resembling a Dirac cone, pointing to excellent charge transport.

As the mechanical properties are correlated with the battery cyclability, we estimate the in-plane stiffness by deriving the direction-dependent (\(\theta\), angle to the armchair direction) Young’s modulus

\[ E(\theta) = \frac{C_{11}C_{22} - C_{12}^2}{C_{11}\sin^4 \theta + C_{22}\cos^4 \theta + \left(\frac{C_{11}^2 - C_{12}^2}{C_{44}}\right)\cos^2 \theta \sin^2 \theta - 2C_{12}\cos^2 \theta \sin^2 \theta} \]

and Poisson’s ratio

\[ \nu(\theta) = \frac{\left(\frac{C_{11} - C_{22} + \frac{C_{11}^2 - C_{12}^2}{C_{44}}}{C_{44}}\right)\cos^2 \theta \sin^2 \theta - C_{12}\sin^4 \theta + \cos^4 \theta}{C_{11}\sin^4 \theta + C_{22}\cos^4 \theta + \left(\frac{C_{11}^2 - C_{12}^2}{C_{44}}\right)\cos^2 \theta \sin^2 \theta} \]

from the linear elastic constants.\textsuperscript{34} The polar diagrams of \(E(\theta)\) and \(\nu(\theta)\) in Figure 2e,f show that Young’s modulus and Poisson’s ratio are almost isotropic in each case. Unlike the electronic properties, the mechanical properties of the C\textsubscript{6}BN monolayers are very similar. The average Young’s modulus and Poisson’s ratio are 309 N/m and 0.178 for C\textsubscript{6}BN-I, 313 N/m and 0.178 for C\textsubscript{6}BN-II, and 315 N/m and 0.183 for C\textsubscript{6}BN-II, which is comparable to graphene (342 N/m and 0.173) and reflects strong bonding and high in-plane stiffness.
where $E_{\text{tube}}$ and $E_{\text{layer}}$ are the total energies per formula unit of a C$_6$BN nanotube and a corresponding C$_6$BN monolayer, respectively, $S_{\text{layer}}$ is the area per formula unit of the C$_6$BN monolayer, and $r$ is the radius of the C$_6$BN nanotube. For each of the C$_6$BN monolayers, nanotubes with six different radii are constructed. The fitting curves are shown in Figure 2g–i and the structural details of the optimized nanotubes are summarized in Table S1. We obtain $B_M$ values of 1.30, 1.36, and 1.38 eV for C$_6$BN-I, C$_6$BN-II, and C$_6$BN-III, respectively, which are lower than those reported for the well-known flexible
2D materials graphene (1.44 eV\textsuperscript{35}) and MoS\textsubscript{2} (9.33 eV\textsuperscript{36}). This indicates enhanced flexibility of the C\textsubscript{6}BN monolayers and, therefore, great potential in wearable electronics.

**Adsorption and Diffusion of K.** Although the C\textsubscript{6}BN monolayers are promising anode materials in terms of their low mass density, high stability, and excellent mechanical properties, spontaneous adsorption of metal atoms is an essential prerequisite. For this reason, we determine the energetically favorable adsorption site of K, i.e., the most likely position of a K atom on the anode material. Based on the different symmetries, nine possible adsorption sites are considered for C\textsubscript{6}BN-I and 16 for C\textsubscript{6}BN-II and C\textsubscript{6}BN-III as shown in Figure 3 (T\textsubscript{a} site on top of an atom; B\textsubscript{at} site on top of a bond; H\textsubscript{at} site on top of the center of a C ring). Unstable adsorption sites show up in the structure optimization by spontaneous diffusion of the K atom to another adsorption site. To determine the affinity of K to a C\textsubscript{6}BN monolayer, we calculate the adsorption energy $E_{\text{ad}} = E_{\text{KC6BN}} - E_{\text{C6BN}} - \mu_K$, where $E_{\text{KC6BN}}$ and $E_{\text{C6BN}}$ are the total energies of a C\textsubscript{6}BN monolayer after and before K adsorption, respectively, and $\mu_K$ is the chemical potential of a K atom from the bcc bulk. The obtained values are summarized in Figure 4a. The negative values indicate spontaneous adsorption of K. It turns out that the H\textsubscript{at} sites are more attractive to K than the T\textsubscript{a} and B\textsubscript{at} sites, which can be attributed

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**Figure 5.** K\textsubscript{x}C\textsubscript{6}BN monolayers: (a) Flowchart of the script used to obtain the lowest energy structure when adding a K atom. No additional sites are found when the number of attempts $n$ approaches 500. (b–d) Maximally potassiated C\textsubscript{6}BN monolayer. (e–g) OCV as a function of the specific capacity with insets showing the formation energy as a function of $x$. (h–j) Variation of the density of states during K adsorption.
To accurately simulate the potassiation process during charging, we add K atoms one after the other to a 3 \times 3 supercell. The lowest energy structure is obtained for each K concentration (1 to 19 K atoms) and C6BN monolayer by the method presented in Figure 3a, considering a total of 3660 structures. The relative stabilities of the intermediate K_{C6BN} structures are then determined relative to the pristine (C6BN) and maximally potassiated (K_{2.11}\text{C6BN}) monolayers in terms of the formation energy $E_f = E_{K,C6BN} - \frac{xE_{K_{2.11}C6BN} + (2.11 - x)E_{C6BN}}{2.11}$ based on total energy calculations. The obtained convex hulls are shown as insets in Figure 5e--g. We find for K adsorption on C6BN-I four points (x = 0.11, 0.22, 1.11, and 2) on the convex hull, i.e., only these four intermediated K_{C6BN} structures are thermodynamically stable. For C6BN-II and C6BN-III there are only three thermodynamically stable intermediate K_{C6BN} structures (as x = 1.11 here is metastable). The intermediate structures during potassiation are shown in Figure S4.

The voltage associated with the potassiation $K_{x}C6BN + (y - x)K^+ + (y - x)e^- \rightarrow K_{y}C6BN$ is

$$V = -\frac{E_{K,C6BN} - E_{K,C6BN} - (y - x)\mu_K}{(y - x)e}$$

which yields the OCV curves shown in Figure 5e--g. For increasing K concentration, the OCV decreases in each case monotonically from an initial positive value. Once a negative value is reached, the K adsorption must stop to prevent dendrite formation. The voltage profile of C6BN-I in Figure 5e shows at the beginning a rapid drop to less than half of the initial value (0.39 V at x = 0; 0.15 V at x = 0.22) and afterward a wide K concentration range with almost constant value (0.13 V at x = 2) in that the battery can provide stable output voltage during discharge. At the K_{2}C6BN to K_{2.11}C6BN transition the voltage switches from positive to negative, suggesting that the maximal K concentration is reached at x = 2 (fully potassiated K_{2}C6BN). The potential profiles of C6BN-II and C6BN-III in Figure 5f, g are very similar to that of C6BN-I. Therefore, all C6BN monolayers can store 2 K atoms per C6BN formula unit, which is almost twice the storage capacity of a graphite anode (1 K atom per 8 C atoms).\textsuperscript{15} We obtain average OCVs for the whole potassiation of 0.16, 0.27, and 0.20 V for C6BN-I, C6BN-II, and C6BN-III, respectively. These low values ensure that there is no risk of dendrite growth (K is stored homogeneously on the C6BN monolayers, see Figure S5) and that the assembled battery can provide high voltage.\textsuperscript{40}

After determining the maximal K concentration, the specific capacity of the half-cell is obtained as $C = \frac{n_F}{3.6M_{C6BN}}$, where $n_F$, $F$, and $M_{C6BN}$ are the number of transferred electrons, Faraday constant, and mass of the C6BN monolayer, respectively. We find that fully potassiated K_{2}C6BN provides a specific capacity of 553 mAh/g, outperforming graphite (279 mAh/g for K_{0.5}C),\textsuperscript{15} Ti_{x}C_{12} (192 mAh/g),\textsuperscript{41} Mo_{x}N_{y} (432 mAh/g),\textsuperscript{42} and phosphorene (433 mAh/g for K_{0.5}P).\textsuperscript{43} The maximal in-plane expansion due to K adsorption is found to be less than 1% for all C6BN monolayers. Together with the absence of structural deformations (Figure 4b--d), this points to robustness of anodes based on C6BN monolayers and, therefore, to excellent cyclability and long service life of the battery.

The conductivity of the anode material determines the Ohmic heating during battery operation. As mentioned previously, K adsorption comes along with electron transfer to the C6BN monolayers. For further evaluation of the consequences, we compare in Figure 5h--j the (partial) density of states of a C6BN monolayer before K adsorption with those of states after adsorption of 1 and 18 K atoms. All pristine C6BN monolayers show a band gap, consistent with our previous discussion. After adsorption of K they turn metallic, because the electrons transferred from K partially occupy the
Conduction band (higher occupation when more K is adsorbed). Therefore, adsorption of K significantly improves the conductivity of the C\textsubscript{6}BN monolayers.

**CONCLUSION**

Motivated by recent synthesis of a C\textsubscript{6}BN monolayer, we predict two new C\textsubscript{6}BN monolayers. They likely can be synthesized by the same experimental method because of structural and energetic similarity combined with good dynamical, thermal, and mechanical stabilities. The C\textsubscript{6}BN monolayers exhibit in-plane stiffnesses comparable to that of graphene while providing enhanced flexibility, which makes them interesting for flexible devices. An investigation of K adsorption demonstrates high specific capacities and low average OCVs for K-ion battery anodes based on C\textsubscript{6}BN monolayers. Also, low K diffusion barriers point to excellent rate performance. The conductivity of the C\textsubscript{6}BN monolayers is significantly improved when K is adsorbed. Overall, our results indicate that C\textsubscript{6}BN monolayers are excellent candidate materials for anodes of K-ion batteries, combining high specific capacity with low cost, high strength, excellent flexibility, low output voltage, excellent rate performance, and improved conductivity. This set of properties calls for experimental efforts to verify the predicted electrochemical performance of C\textsubscript{6}BN monolayers.

**ASSOCIATED CONTENT**

1. Supporting Information
   The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acsami.0c09451.
   Structural details of the optimized C\textsubscript{6}BN nanotubes; total energy of C\textsubscript{6}BN-I for different k-meshes; top and side views of the unit cells of C\textsubscript{6}BN-II and C\textsubscript{6}BN-III; thermal stability of the C\textsubscript{6}BN monolayers at 1200 K; intermediate structures during potassiation; maximally potassiated C\textsubscript{6}BN monolayers at 300 K. (PDF)

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**Notes**
The authors declare no competing financial interest.

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