Large Magnetoresistance in Scandium Nitride Magnetic Tunnel Junctions Using First Principles

Suyogya Karki, Vivian Rogers, Priyamvada Jadaun, Daniel S. Marshall, and Jean Anne C. Incorvia*

The state-of-the-art magnetic tunnel junction, a cornerstone of spintronic devices and circuits, uses a magnesium oxide tunnel barrier that provides a uniquely large tunnel magnetoresistance at room temperature. However, the wide bandgap and band alignment of magnesium oxide-iron systems increases the resistance-area product and creates variability and breakdown challenges. Here, the authors study using first principles narrower-bandgap scandium nitride (ScN) transport properties in magnetoresistive junctions in comparison to magnesium oxide. The results show a high magnetoresistance in Fe/ScN/Fe via $\Delta_1$, and $\Delta_2$ symmetry filtering with low wave function decay rates, suggesting scandium nitride could be a new barrier material for spintronic devices.

1. Introduction

Magnetic tunnel junctions (MTJs) are basic building blocks for emerging spintronic devices, including for spin transfer torque-magnetic random access memory,[1] a leading emerging non-volatile memory that is steadily transitioning into production, as well as for magnetic logic-in-memory[2,3] and neuromorphic computing[4,5] applications. An MTJ consists of a thin insulating tunnel barrier sandwiched between two ferromagnetic (FM) electrodes. When a current is passed across the barrier, parallel (P) magnetization of the two electrodes provides a higher density of states for the majority spin electrons to tunnel across, giving a low resistance, $R_P$, state. When the magnetization of the two electrodes is antiparallel (AP), the device is in a high resistance, $R_{AP}$, state. These two states can be used as 1’s and 0’s for memory and logic applications. The MTJ is characterized by the tunnel magnetoresistance ($MR$), $TMR = \frac{R_{AP} - R_P}{R_P} \times 100\%$, and the resistance-area product $RA = R_P \times A$, where $A$ is the cross-sectional area of the junction.

Progress in MTJ devices has been driven by materials revolutions. Spin-dependent tunneling behavior was first implemented in amorphous aluminum oxide ($Al_2O_3$) tunnel junctions,[6] which have shown a room temperature $TMR$ up to $\approx 70\%$. About 10 years later, a larger $TMR$ was measured in magnesium oxide (MgO) barriers,[7] showing $TMR$ above $600\%$[8] at room temperature in experiments. MgO has been the tunnel barrier of choice for over 10 years because of its unique spin transport properties: MgO [001] can lattice match to Fe [001] to prevent mixing of electron states as they tunnel across the barrier and selectively filters out all tunneling symmetries except the $\Delta_1$ band in Fe. Fe’s $\Delta_1$ band is highly spin-polarized and has no available states at the Fermi level in the minority spin, which allows for a theoretically ultra-high magnetization-dependent tunneling via Bloch waves with small transverse momentum.[9]

However, there are challenges to using MgO that hinder MTJs and their associated technologies from competing with other emerging memories.[10] A major challenge is that very thin tunnel barriers are necessary. The MgO layer is grown $1.5 \text{ nm}$ thick to have a reasonably low $RA$. This is due to both the wide $7.8 \text{ eV}$ bandgap of MgO and the metal-insulator band alignment. Pinholes present in this thin layer can create a path for current and degrade the $MR$, and when so thin, slight variations of the thickness across a wafer create variations in the $MR$ and $RA$.[11,12] In addition, an FeO interlayer is created upon annealing at higher temperatures, decreasing expected $MR$ values in the experiment.[13] This makes MgO MTJs a challenge to grow, especially compared to competing technologies such as resistive random-access memory. It is also a hindrance for advanced applications of MTJ devices in artificial intelligence and neuromorphic computing, where current may be applied across the tunnel barrier often during real-time adaptation to the environment and where novel switching methods may be used that require higher current across the barrier, causing device breakdown.[14,15] These challenges lend credence to investigating alternative materials to MgO that can have similar symmetry-filtering transport properties with a narrower bandgap, although no materials have been able to compete with the $MR$ of MgO to-date at room temperature.

Here, we study using first principles the tunneling properties of scandium nitride (ScN) to understand the material’s transport
characteristics and determine if MTJs using ScN can achieve high MR. ScN is chosen for this study because it has a narrower bandgap than MgO (indirect transition from the X to Γ point of 0.9–1.6 eV and direct gap at the X point of 2–2.9 eV) and it has a similar rock salt crystal structure to MgO. ScN[001] is face-centered cubic (FCC) with lattice constant a = 4.501 Å compared to MgO[001], also FCC with a = 4.212 Å. ScN is a group IIIB transition metal nitride and has not been widely used in device applications, but has found niche uses in GaN crystal growth and radio frequency devices.

There is ongoing research in developing barrier materials with large MR ratios to try to compete with MgO, largely in the class of Mg oxide alloys. In one simulation study, ZnO with rock salt structure, bandgap 2.132 eV at the Γ point, and indirect gap of 0.913 eV showed MR = 446% and RA = 0.0468 Ω-μm². There is also recent interest in exploring alternate electrode materials for higher spin polarization; one such example is the use of Heusler compounds for both electrodes and barrier materials. A recent work on NiMnSb-MgO junctions predicted high MR > 10⁴.

To our knowledge, no work has investigated ScN MTJs.

We investigate the complex band structure of ScN, as well as electron transport in Fe/ScN/Fe MTJs, to understand ScN’s properties as a spin filter using density functional theory (DFT) and plane wave conductance techniques. Figure 1a shows the converged ScN lattice with a rock salt crystal structure using visualization software VESTA. Depicted in Figure 1b, supercells of both Fe/ScN[001]/Fe and Fe/MgO[001]/Fe systems are created for t = 3–8 atomic layers of the barrier region to compare the ScN and MgO behavior. In x and y, the unit cell is repeated to infinity; in z the Fe leads extend to infinity in both directions.

To interface with Fe electrodes, the ScN and MgO unit cells are rotated by 45° around the z direction such that the anion atoms (O or N) in the barrier region are positioned directly above the Fe at the interface. After this rotation, the lattice parameter is constrained to the experimental lattice constant of Fe (2.866 Å) in the x and y directions. This induces a 3.9% in-plane compressive strain in the barrier to match the experimental lattice parameter of MgO (4.212 Å), and for ScN the experimental lattice parameter of 4.501 Å is compressed by 11% to match with the leads. These supercells are relaxed using the Vienna ab-initio simulation program (VASP) with molecular dynamics. The wave functions and resulting conductance of the system are calculated using the Quantum Espresso package.

The spin up (T↑) and spin down (T↓) transmission probabilities, that is, the probability for transmitting an electron that enters the channel, is calculated. The conductance is then calculated using the Landauer formula G = e²/h (T↑ + T↓) and resulting conductance of the system are calculated using the Quantum Espresso package.

2. Results

Using the Perdew–Burke–Ernzerhof (PBE) pseudopotential, Figure 2a shows the band structure with an indirect gap of 0 eV. With the additional Hubbard potential of 4.5 eV added to the 3d orbital of Sc, in Figure 2b there is a direct gap at the Γ point of 2.99 eV, a direct gap at the X point of 2.28 eV, and an indirect Γ-X gap of 1.31 eV. These results are in agreement with a previous DFT+U simulation, which showed the ScN band structure having a direct gap at the Γ point of 3.39 eV and a direct gap at the X point of 1.55 eV. The calculation is also comparable to experimental values, where gaps are observed at the Γ point of 3.8 eV, at the X point of 2.4 eV, and an indirect Γ-X gap of 1.3 ± 0.3 eV.

The complex band structures of bulk ScN (Figure 2c) and bulk MgO (Figure 2d) are sampled at the Γ and X points. The intersection of the Fermi energy (E_F) and the complex bands shows the rate of decay of the particular symmetry band with respect to real
Figure 2. Band structure. a) Band structure of ScN with direct gap at the Γ point of 2.43 eV. b) Band structure of ScN with 4.5 eV Hubbard potential added to the 3d orbital of Sc. The complex bands of c) ScN and d) MgO are shown, sampling into imaginary k space from the Γ and X points with the symmetry-resolved real bands set in-between.

For MgO, Figure 2d shows Im(k) = 0.21 2/π at the Γ point, showing MgO’s Δ1 band has the slowest decay rate compared to the other bands and thus dominates transmission as expected. For ScN, Figure 2c shows a comparatively low decay rate of the Δ1 band at the Γ point, as well as a low decay rate of the Δ2’ band at the X point, implying both Δ1 and Δ2’ are likely to contribute to transport. The low decay rates suggest that the resistance could be lower in ScN systems compared to MgO. Depending on the band alignment of ScN with the electrodes, one of these two symmetries may be favored. As shown in the Supporting Information, the Δ2’ band in Fe has spatial dependence in the direction of current propagation at the Fermi energy in the majority spin, but little momentum in the minority spin, and could also contribute to spin polarization.

In Figure 3 the transmission probability T for Fe/ScN(t = 6)/Fe MTJs (top row) and Fe/ScN(8)/Fe MTJs (middle row) is compared to Fe/MgO(6)/Fe MTJs (bottom row) for both spin channels and both magnetic orientations of the Fe electrodes. The plots show the transmission probability for each kx and ky point in the supercell Brillouin zone centered at the Γ point, using a 200 × 200 k-grid. In the transmission plot for the majority P channel for 6 layers of ScN, Figure 3a, conduction occurs at the center of the Brillouin zone and along the X and M points of the tetragonal supercell. The conduction band minimum in the ScN band structure is at the X point and the ScN lattice has been rotated 45° around the z axis for the supercell. As expected, this is reflected in the high transmission lobes around the supercell M points. In the transmission plot for the majority P channel for 8 layers of ScN, Figure 3e, conduction occurs at the center of the Brillouin zone and around the Γ point, with no transmission lobes around X and M points. The conduction differences seen in t = 6 and t = 8 MTJs can be attributed to different band alignments of the Fe electrodes relative to the ScN bandgap. Since DFT is not the best predictor of band alignments, which is exacerbated in lower bandgap systems, here we include results for various thicknesses and draw more general conclusions, independent from the exact band alignment, about the expected behavior. See Supporting Information for additional plots of the layer-resolved local density of states (LDOS) for every layer around the junction center, for t = 5–8.

In comparison, the MgO majority P channel, Figure 3i, shows a broad peak centered at the Γ point via the Fe Δ3 band. Figures 3b,f, and j show transmission plots of the minority channel when the electrode magnetization is parallel, with orders-of-magnitude reduced transmission compared to majority spins.

Figures 3c,d show the conduction through ScN (t = 6) when the electrodes have AP magnetization, similarly in Figures 3g,h for t = 8, and compared to MgO AP in Figures 3k,l. Compared to Figures 3a,b the transmission in the spin up and spin down channels in the 6 layers AP ScN system show a much broader peak around the Γ point with lobes around the X point. For ScN (t = 8) the transmission peaks for both channels in AP are primarily seen around the Γ point. In MgO, the transmission peaks
Figure 3. \( k - \text{resolved transmission probability.} \) a–d) Transmission probability through Fe/ScN (6)/Fe MTJs, where \( t \) is in atomic layers. e–h) Transmission probability through Fe/ScN (8)/Fe MTJs. i–l) Transmission probability through Fe/MgO (6)/Fe MTJs. a, e,i) Majority channel for parallel alignment of Fe electrode magnetizations. b,f,j) Minority channel for parallel alignment of Fe electrode magnetizations. c,g,k) Majority channel (up of input electrode) for antiparallel alignment of Fe electrode magnetizations. d,h,l) Minority channel (down of input electrode) for antiparallel alignment of Fe electrode magnetizations. Color label indicates the transmission probability at each \( k \) point. Plots are centered on the \( \Gamma \) point with \( X \) and \( M \) points labeled in (i).

for both channels are primarily seen around the \( \Gamma \) point, with most transmission around the \( X \) point filtered out compared to the \( P \) minority channel.

The results for Fe/MgO/Fe agree with previous work\(^9\) and give confidence to the validity of the model. As expected, MgO shows high spin filtering: the majority channel dominates conductance compared to the minority channel, leading to the high \( MR \) seen in MgO MTJs. Promisingly, ScN shows similar spin filtering properties. For example, for \( t = 6 \) layers, integrating the transmission over the Brillouin zone, the majority channel in the parallel magnetized electrodes shows a 75× higher conductance compared to the minority channel. Also, the conductance is 120× higher in the parallel magnetized electrodes compared to the antiparallel electrodes, indicating that ScN MTJs can also achieve high \( MR \).

To understand which Bloch states contribute to spin polarized transport, we sample the scattering states versus \( z \) for the highest conductance electron channels in the parallel-magnetized 6 and 8 layer ScN systems. Figure 4a,b shows the conductance at the \( (k_x = 0.02, k_y = 0.05) \) transmission spike near the center of the Brillouin zone for majority (Figure 4a) and minority (Figure 4b) spin for the 6-layer system. Figure 4a shows that \( \Delta_1 \) has high conductance for majority spins while \( \Delta_1 \) shows a modest decrease across the barrier. The two next-highest channels are mixed states and greatly decrease in amplitude across the barrier. Using PWCOND, the eigenchannel wave functions can be obtained at certain \( k \) points; however, it sorts them by transmission value in the symmetry eigenbasis and does not characterize the symmetry itself. The transmissions were cross-referenced with the known symmetries of the square lattice which clearly identified \( \Delta_1 \) and \( \Delta_2' \) symmetries for the dominant eigenchannels. Using the same method, the lower transmission value eigenchannels clearly showed mixed states, but this method cannot pick out the exact mixed states. In Figure 4b for minority spin, two mixed states are observed and decrease across the barrier. Similar behavior is seen in the other transmission spikes that dominate transmission across the Brillouin zone (see Supporting Information).

Looking at the 8-layer system and picking out a transmission spike at \( k_x = 0.00, k_y = 0.195 \), Figure 4c shows the conductance in the majority spin is dominated by the \( \Delta_1 \) channel only. For the minority spin, Figure 4d, two mixed states are observed which decrease across the barrier. These results show that depending on the thickness of the ScN barrier layer and Fe-ScN band alignment, spin-polarized transmission is expected through either \( \Delta_1 \) or \( \Delta_2' \) channels. This analysis was done for the \( P \) configuration, but not the \( AP \) configuration. When modeling the \( AP \) configuration, a discontinuity in magnetization is created so that the Fe atoms in the barrier supercell match up to the semi-infinite leads as they would in bulk Fe. This makes it difficult to extract the symmetry states from the \( AP \) configuration.

The conductance calculations were carried out for \( t = 3–8 \) layers, summarized in Table 1. The \( t = 4 \) layers system had unstable
molecular dynamics convergence and thus was not calculated. It is seen that in the ScN systems in Table 1, $\text{MR} = 108\text{–}11\text{ 800}\%$ showing that ScN can demonstrate large $\text{MR}$. In comparison, the Fe/MgO/Fe system in Table S2, Supporting Information, $\text{MR} = 480\text{–}41\text{ 800}\%$, in agreement with previous simulation results. We do not expect real devices to have fluctuations in $\text{MR}$ with thicknesses, as the barrier would be thicker than few atomic layers. Our model validates that spin-dependent tunneling is achieved in the ScN MTJs with additional tunneling mechanisms compared to MgO MTJs. While the exact $\text{MR}$ values and band alignments may not be predictive, the overall behavior of spin polarization via $\Delta_1$ and $\Delta_2'$ channels and resulting high $\text{MR}$ in ScN MTJs is clear.

It is observed in Table 1 for Fe/ScN/Fe MTJs there is a wide range of magnetoresistance and a non-exponential decay of conductance in each channel with respect to barrier thickness, motivating an explanation for the deviation from the expected relationship seen in MgO MTJs. The breakdown of crystallinity due to lattice mismatch of ScN and Fe electrodes and the unique $\Delta_2'$ conduction through the X point could explain this behavior. For the majority channel in MgO, most of the conduction is due to tunneling states with little transverse momentum at the $\Gamma$ point. In ScN, there are additional tunneling states around the X points, which have electron plane waves of a higher spatial frequency than those around the $\Gamma$ point. This suggests a strong layer-dependent wave function interference within the barrier region, as seen in the interface resonance in the MgO’s minority spin electron transport.[9]

In the molecular dynamics simulation, the ScN lattice is compressed in $x$ and $y$ to match the Fe electrodes due to the large

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**Figure 4.** Scattering states versus $z$, a) for $t = 6$ layers majority spin sampled at $k_x = 0.02$ and $k_y = 0.05$ (identified by white arrows) and b) minority spin. c) For $t = 8$ layers majority spin sampled at $k_x = 0.00$ and $k_y = 0.195$ and d) minority spin. Dotted lines delineate the barrier region with Fe electrodes to left and right.

**Table 1.** ScN MTJ conductance and magnetoresistance. For each barrier layer number studied, conductance values are shown for parallel ($G_p$) and antiparallel ($G_{AP}$) alignment in units of $[Ω^{-1}]$. Majority and minority channel conductance is also shown, in parallel and antiparallel alignment of the electrodes $G_p^\uparrow$, $G_p^\downarrow$, and $G_{AP}$, in units of $[e^2h^{-1}]$. The corresponding $\text{MR}$ is calculated.

| Layers          | $G_p^\uparrow$ [$e^2h^{-1}$] | $G_p^\downarrow$ [$e^2h^{-1}$] | $G_p$ [$Ω^{-1}$] | $G_{AP}$ [$e^2h^{-1}$] | $G_{AP}$ [$Ω^{-1}$] | MR ratio [%] |
|-----------------|-------------------------------|---------------------------------|------------------|-------------------------|---------------------|--------------|
| Fe/ScN(3)/Fe    | $6.64 \times 10^{-3}$         | $2.73 \times 10^{-3}$          | $1.81 \times 10^{-7}$ | $1.19 \times 10^{-3}$   | $7.15 \times 10^{-4}$ | 153          |
| Fe/ScN(5)/Fe    | $2.09 \times 10^{-4}$         | $8.66 \times 10^{-5}$          | $5.71 \times 10^{-4}$ | $7.09 \times 10^{-3}$   | $2.74 \times 10^{-9}$ | 108          |
| Fe/ScN(6)/Fe    | $6.44 \times 10^{-3}$         | $8.63 \times 10^{-5}$          | $1.26 \times 10^{-2}$ | $2.74 \times 10^{-5}$   | $1.06 \times 10^{-9}$ | 11 800       |
| Fe/ScN(7)/Fe    | $2.96 \times 10^{-3}$         | $9.62 \times 10^{-4}$          | $7.57 \times 10^{-4}$ | $9.73 \times 10^{-5}$   | $3.76 \times 10^{-9}$ | 1920         |
| Fe/ScN(8)/Fe    | $9.30 \times 10^{-3}$         | $2.64 \times 10^{-4}$          | $1.83 \times 10^{-2}$ | $6.97 \times 10^{-5}$   | $2.69 \times 10^{-9}$ | 6750         |
We have shown from first principles that Fe/ScN/Fe MTJs have many of the desirable spin-dependent transport properties of Fe/MgO/Fe junctions, namely a low $\Delta t$ decay rate through the $\Gamma$ point, but with additional conduction pockets through the $\Delta_{\gamma}$ symmetries at the X point. We have shown this leads to a high MR, competitive with that in Fe/MgO/Fe. These results indicate that ScN could be an exciting new material for MTJ devices, in a field where few alternative materials to MgO have been developed. The work motivates experimental studies, exploration of better lattice-matched electrodes for ScN, study of other lower bandgap materials for advanced MTJ applications, investigation of effects of thermionic emission, and understanding of how the nitrogen-based barrier can affect device properties compared to traditional oxide-based tunnel barriers.

4. Experimental Section

The MTJ supercell was created for various layer numbers ($t$) for both ScN and MgO systems. The systems with odd $t$ had 6 Fe atoms on the bottom side and 5 Fe atoms on the top side of the supercell. For the $t = 6$ systems, 6 atoms of Fe were placed on each side of the barrier to maintain the periodicity of the system and to ensure a match with the leads in conduction. The supercells were relaxed using the VASP with molecular dynamics such that all forces were $< 0.01$ eV Å$^{-1}$. The convergence was also done for the total free energy and the band structure energy so that the change between two timesteps was $< 10^{-5}$ eV. The authors were aware that for high spin-orbit coupling systems a higher convergence criterion was necessary. In their system they had neglected the spin-orbit perturbations; thus, a convergence criterion of $1 \times 10^{-5}$ eV should be sufficient, as shown in other works in literature. In the simulation for ScN $t = 4$ layers there was instability in the molecular dynamics convergence while using the same convergence criteria as the other systems. This was due to problems during reading of the CHGCAR file in the molecular dynamics simulation. Starting the charge density from scratch solved the issue, but they did not move forward in the conduction stage as it required additional time and resources. Using Perdew–Burke–Ernzerhof (PBE) functionals, the Fe/ScN/Fe and Fe/MgO/Fe supercells were converged using these cut-offs with an $11 \times 11 \times 11$ k point mesh. The converged supercell atomic positions were then copied into Quantum Espresso to generate wave functions of the supercells and perform transport calculations.

To generate the wave functions and calculate the complex bands and unit cell conductance, PWscf and PWcond were used from the
Quantum Espresso package. The complex bands were generated with a 4-atom tetragonal unit cell for both bulk ScN and MgO using USPP PBE scalar-relativistic pseudopotentials, with the symmetry-resolved real bands sampled in the direction of conduction. Cutoffs of 50 and 500 Ry were used for the wave function and charge density cutoffs. In quantum espresso for complex band calculations a different projection method known as pseudo potential method required a +U of 6 eV. A range of +U was used to match the gaps with experiment, and they found 8 eV was optimum for this projection technique.

After minimizing the energy of the MTJ unit cells in VASP, a PWscf self-consistency field (SCF) calculation was run using Scalar-relativistic PBE functionals with projector augmented wave potentials to generate the wave functions.[35] For all supercells, 64 and 782 Ry were used for the wave function and charge density cutoffs, respectively. Marzari–Vanderbilt smearing[36] was used with a broadening parameter of 0.02. For the SCF calculation, an 11 × 11 × 1 Monkhorst-Pack grid was used. The electronic convergence has a criterion of 1 × 10^{-8} Ry. For the systems with parallel magnetization of the leads, both leads were magnetized in the +z direction, with the average magnetization of the Fe atoms converging to roughly 2.3 μB. For the systems with antiparallel lead magnetization, the atomic positions of the parallel alignment system were duplicated in the +z direction to create a Fe/Barrier/Fe-Fe/Barrier/Fe supercell. The far bottom and top Fe regions were magnetized in +z, and the middle Fe region was magnetized in −z, where the supercell would be cut in half for conduction calculations. This avoided modeling a discontinuity in magnetization to ensure that the Fe atoms in the barrier supercell matched up to the semi-infinite leads as they would in bulk Fe. The wave functions of the electrode unit cells were generated using the same parameters, except an 11 × 11 × 1 k-grid was used to reflect the cubic nature of the Fe unit cells in the bulk material.

In the SCF stage for the ScN systems, a DFT+U Hubbard offset of 4.5 eV was applied to the Sc atoms via the atomic projection method to match the bandgap with experimental values. They found this value by sweeping the Hubbard offset from 3 to 6 eV for bulk ScN and examining the bandgap with experimental values. They found this value by sweeping the Hubbard offset from 3 to 6 eV for bulk ScN and examining the bandgap with experimental values. They found this value by sweeping the Hubbard offset from 3 to 6 eV for bulk ScN and examining the bandgap with experimental values. They found this value by sweeping the Hubbard offset from 3 to 6 eV for bulk ScN and examining the bandgap with experimental values. They found this value by sweeping the Hubbard offset from 3 to 6 eV for bulk ScN and examining the bandgap with experimental values. They found this value by sweeping the Hubbard offset from 3 to 6 eV for bulk ScN and examining the bandgap with experimental values.

For the systems with antiparallel lead magnetization, the atomic projectors for Hubbard +U calculations, which requires a larger window of 8 Ry was used for reducing the 2D plane wave basis set in transmission for the smaller systems, though the 7-layer systems were reduced to 6 Ry to improve stability. Both were converged to an accuracy of 10^{-8} Ry. The transmission was resolved with a 200 × 200 k-grid in x and y; a finely grained k-grid proved important for accurately capturing fine spikes in transmission.

The PWCOND complex bands calculation requires the implementation of Scandum’s built-in pseudopotential projectors as opposed to the atomic projectors for Hubbard +U calculations, which requires a larger value of U to approach a similar band structure.[19] With this applied ‘pseudo’ Hubbard correction, the bandgaps were not able to match with experimental values, but still allow analysis of the tunneling mechanisms in ScN MTJs. The conduction and real band structure simulations in the rest of the paper was using the ‘atomic’ method with a +U of 4.5 eV and unaffected by this, matching experimental results for ScN.

Supporting Information
Supporting Information is available from the Wiley Online Library or from the author.

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Conflict of Interest
The authors declare no conflict of interest.

Author Contributions
S.K. and V.R. carried out the simulations with assistance from P.J. and prepared the manuscript. D.M. provided ideas and discussions of importance to the work. J.A.C.I. created, led, and supervised the work and manuscript.

Data Availability
The datasets generated during and/or analyzed during the current study are available from the corresponding author on reasonable request.

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