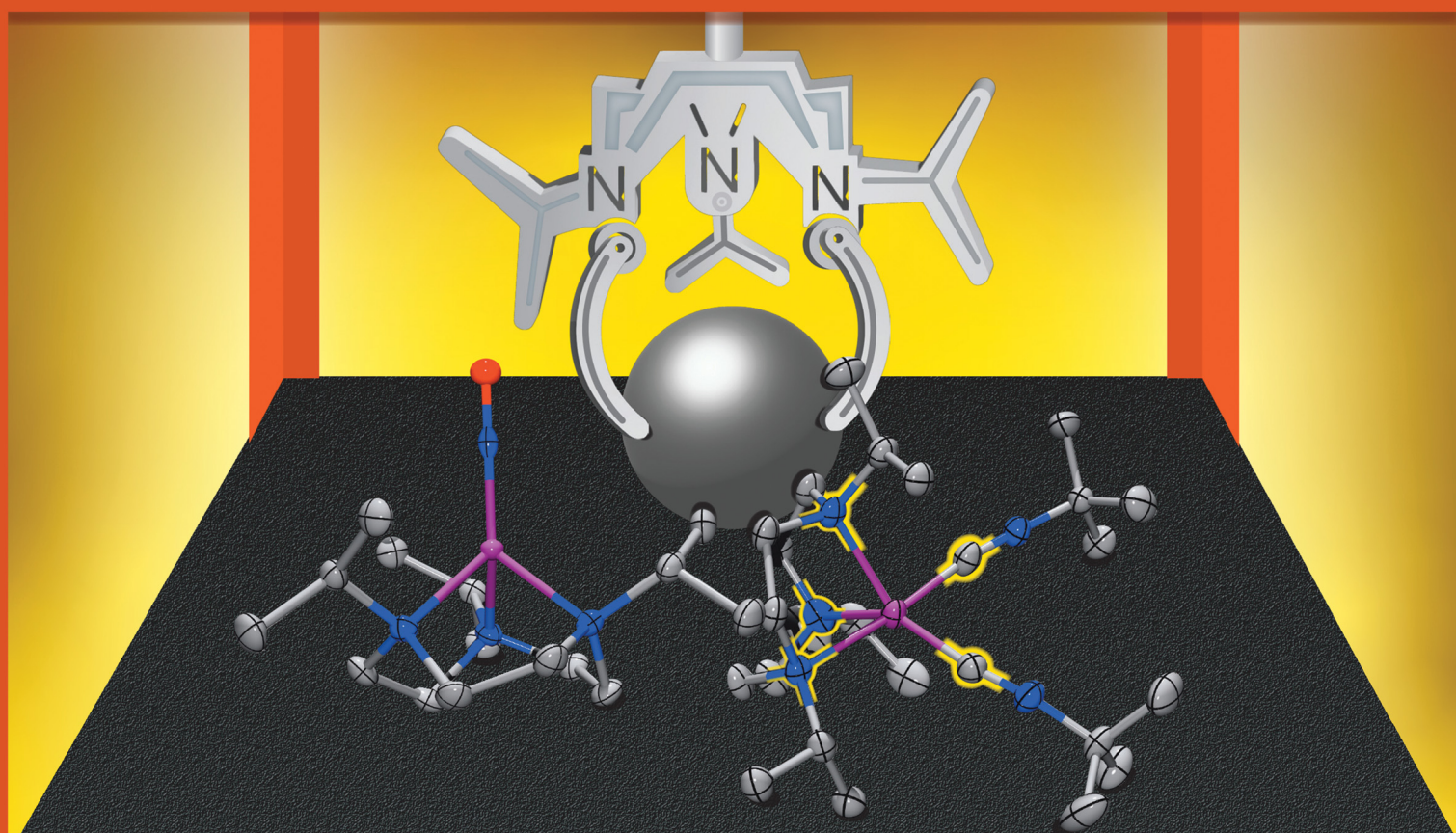


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A five-coordinate Ni(I) complex supported by 1,4,7-triisopropyl-1,4,7-triazacyclononane†

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An isolated Ni(II)-nitrosyl complex supported by the bulky tridentate 1,4,7-triisopropyl-1,4,7-triazacyclononane (iPr₃TACN) ligand was obtained from the reaction of a Ni(II) dimethyl complex with NOPF₆, suggesting the *in situ* formation of a Ni(I) species that reacts with the resulting NO product. Use of a π-acceptor ancillary isocyanide ligand led to the isolation and characterization of an uncommon 5-coordinate Ni(I) complex supported by the iPr₃TACN ligand and *tert*-butylisocyanide.

Ni complexes are known to be efficient catalysts for various types of cross-coupling reactions. Although many Ni(0)/Ni(II) species have been reported as intermediates Ni-mediated catalysis, newer studies suggest that their odd-electron Ni(I)/Ni(III) counterparts are also viable catalytic intermediates.^{1–4} More recent studies have focused on accessing and isolating rare Ni(III) organometallic complexes; nevertheless, the related organometallic Ni(I) species are sometimes overlooked.²

Several Ni(I) coordination complexes have been reported,⁵ and such species are essential in the catalytic process as they can undergo radical or oxidative addition of various electrophiles, key steps in a catalytic cycle.^{6–10} For example, there are only a few examples involving an oxidative addition of an alkyl or aryl halide to a Ni(I) metal center.^{11–16} While the latter complexes were also supported by N-based ligands, none of them employed a macrocyclic ligand. Our group has previously reported the isolation of Ni complexes in the +2, +3, and +4 oxidation states stabilized by various N-based macrocyclic ligands. In these systems a Ni(I) intermediate is commonly proposed to form *in situ* upon the reductive elimination of C–C bond formation products, yet due to the hard-donating nature of the employed ligands we have never observed or isolated a Ni(I) complex.^{17–25} In our efforts to isolate low-valent Ni(I)

complexes we have employed the soft-donor macrocyclic ligand *P,P'*-ditertbutyl-2,11-diphosphonito[3.3](2,6)pyridinophane (N2P2) in combination with isocyanides,²⁶ yet the use of N-donor macrocycles to stabilize Ni(III) species has remained elusive. More recently, we have employed the bulky tridentate N-donor ligand 1,4,7-triisopropyl-1,4,7-triazacyclononane (iPr₃TACN) to explore the oxidatively induced reactivity of the (iPr₃TACN)Ni(II)Me₂ (**1**) complex. Herein, we report the use of iPr₃TACN and a π-acceptor ancillary isocyanide ligand that leads to the isolation and characterization of an uncommon 5-coordinate Ni(I) complex supported by the iPr₃TACN ligand and *tert*-butylisocyanide.

Interestingly, during the oxidatively induced reactivity studies of **1**, the use of 0.9 equiv. NOPF₆ leads to the formation of [(iPr₃TACN)Ni(II)NO]PF₆ (**2**) as a violet powder in 73% yield (Fig. 1).²⁷ X-Ray quality crystals were obtained and the solid-state structure was determined to reveal a four-coordinate Ni(II) tetrahedral complex with a geometry index of τ₄ = 0.74. Examining the Ni–N bond distances, three equivalent Ni–N bonds

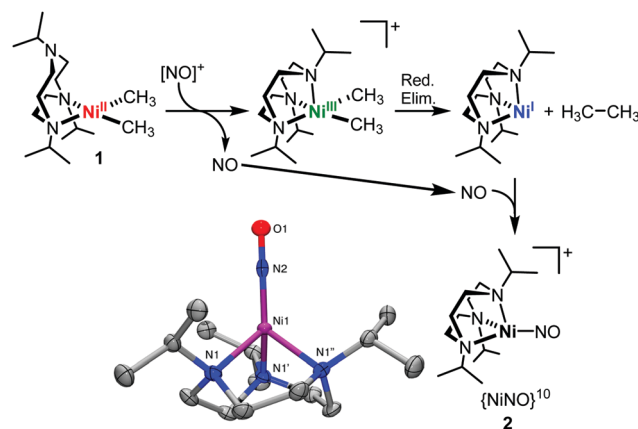


Fig. 1 Synthetic scheme and mechanism for the formation of **2** and the ORTEP representation of its solid-state structure with 50% probability ellipsoids. Hydrogen atoms and anions omitted for clarity. Selected bond lengths (Å): Ni1–N1, 2.042(2); Ni1–N2, 1.677(4); N2–O1, 1.123(5). Selected bond angle (°): Ni1–N4–O1, 180.0.

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with a length of 2.042 Å were observed. In addition, the Ni–N_{NO} bond distance of 1.646 Å and the N–O bond length of 1.12 Å are slightly shorter than other Ni(II)–NO complexes reported in the literature,^{28–31} but consistent with a N≡O triple bond character that is further confirmed by the linear Ni–N≡O interaction with a Ni1–N4–O1 bond angle of 180°. The IR spectrum of **2** reveals a distinctive N≡O bond stretch at 1770 cm⁻¹, which is well within the range for a M–N≡O triple bond.^{28,29,32} Previous studies with tridentate N-based ligands such as the sterically hindered Tp (hydrotris(pyrazolyl)borate) ligand have proven successful in the isolation and characterization of tetrahedral metal-nitrosyl complexes.^{33,34} However, to the best of our knowledge, there are no examples of nitrosyl complexes supported by redox innocent N-based tridentate ligands.³¹ Furthermore, the ¹H NMR of a solution of **2** reveals a diamagnetic spectrum, which supports the presence of a {NiNO}¹⁰ species based on the classification of Enemark and Feltham,³² and thus **2** can be viewed as a Ni(0)–NO species if the nitrosyl ligand is treated as NO⁺, or a Ni(II)–NO species if the nitrosyl ligand is treated as NO⁻ (Fig. 1).³⁵

Based on the observed reactivity of **1** with NOPF₆ and the formation of **2** in high yield, we propose the following mechanism: one-electron oxidation of **1** by NOPF₆ followed by rapid reductive elimination of ethane from the transient Ni(III)Me₂ intermediate would generate a Ni(I) species (Fig. 1). Although such a Ni(I) was not observed by Electron Paramagnetic Resonance (EPR) even when the reaction was performed at low temperature, such a species should rapidly react with the NO by-product, formed from the reduction of NO⁺, to generate **2** (Fig. 1). Similarly, Warren *et al.* have previously reported the synthesis of a reactive β-diketiminato Ni(I) complex that reacts directly with NO to generate a {NiNO}¹⁰ complex.²⁹ Interestingly, the reaction of **1** with 1–1.1 equiv. of NOPF₆ led to the formation of a mixture of **2** and the blue complex [(iPr₃TACN)Ni(II)(NOCH₃NO)]PF₆. The latter *N*-methyl-*N*-nitrosohydroxylaminato complex could not be obtained purely for full characterization, yet characterization by single-crystal X-ray diffraction confirms its identity (Fig. S16, ESI†). These results are consistent with the report of Warren *et al.* in which an *N*-ethyl-*N*-nitrosohydroxylaminato complex was observed in addition to the Ni-nitrosyl complex, and for which a mechanism involving a reaction between a Ni(I) complex and NO was also proposed,²⁹ and thus providing further support for our proposed mechanism to yield **2** (Fig. 1). Overall, the ability of the iPr₃TACN ligand to stabilize a “Ni(0)–NO⁺” species, as well as a potential Ni(I) intermediate, prompted us to further pursue the isolation of a (iPr₃TACN)Ni(I) complex by employing ancillary π-acceptor ligands that are commonly used to stabilize low-valent metal centers, such as *tert*-butyl isocyanide (tBuNC).⁵

We first synthesized the bis-solvento Ni(II) complex [(iPr₃TACN)Ni(II)(MeCN)₂](PF₆)₂ (**3**) via halogen abstraction from a previously reported (iPr₃TACN)Ni(II)Cl₂ complex.^{36,37} Addition of 2.1 equiv. of TlPF₆ to (iPr₃TACN)Ni(II)Cl₂ in MeCN yielded a blue solution from which **3** was obtained in 94% yield as a blue crystalline solid. The solid-state structure of complex **3** reveals a 5-coordinate Ni(II) center with a pseudo-square pyramidal

geometry and a geometry index of τ₅ = 0.46 (Fig. 3a). The 5-coordinate geometry is supported by three N-donors from the iPr₃TACN ligand and coordination of two MeCN molecules, with Ni–N_{ave} bond distances of 2.072 Å for the iPr₃TACN ligand and 2.051 Å for the nitrile ligands, respectively. In contrast, the methyl TACN (Me₃TACN) analogue adopts an octahedral geometry allowing a third MeCN ligand to coordinate to the metal center to give complex [(Me₃TACN)Ni(II)(MeCN)₃](BF₄)₂,³⁸ and thus highlighting the increased steric bulk of the iPr₃TACN ligand.

We then prepared [(iPr₃TACN)Ni(II)(CN^tBu)₃](PF₆)₂ (**4**) upon the addition of 3.1 equiv. of tBuNC to a suspension of complex **3** in THF, to yield a pale green solid product in 94% yield (Fig. 2). X-Ray quality crystals of **3** were obtained from vapor diffusion of Et₂O into a MeCN solution, and the solid-state structure reveals an octahedral Ni(II) center with the iPr₃TACN ligand coordinating in a κ³ fashion with an average Ni–N bond length of 2.125 Å (Fig. 3b). To our surprise, the sterically encumbered complex had three tBuNC molecules coordinated to the metal center, with an average Ni–CNR distance of 1.946 Å and a C≡N bond length of 1.112 Å, which is consistent with previously reported mononuclear Ni(II)–CNR bond distances of similar complexes deposited in the Cambridge Crystal Database (CCDC).³⁹ Cyclic voltammetry (CV) studies reveal a chemically accessible redox couple at E_{1/2} = -0.92 V vs. Fc⁺/Fc, with was assigned to Ni^{II}/Ni^I redox process (Fig. 4).

Addition of cobaltocene to a suspension of **4** in THF yielded the thermally stable [(iPr₃TACN)Ni(I)(CN^tBu)₂](PF₆) (**5**) in 79% yield. X-Ray quality crystals with a dichroic yellow/green color were obtained from the vapor diffusion of Et₂O into a concentrated MeCN solution. Excitingly, the solid-state structure revealed an unusual 5-coordinate Ni(I) complex adopting a distorted trigonal bipyramidal/square pyramidal structure with a geometry index of τ₅ = 0.53 (Fig. 5). Similar to its Ni(II) analogue, iPr₃TACN ligand coordinated in a κ³ fashion to the Ni center in **5**, yet a slight elongation was observed for with an average Ni–N bond length of 2.199 Å. Furthermore, although we expected a low-coordinate Ni(I) center, we were surprised that two tBuNC molecules coordinate to the metal center with an average Ni–CNR distance of 1.894 Å, which is consistent with previously reported Ni(I)–CNR bond distances.^{40–42} However, we note that the reported Ni(I)–CNR complexes are limited to those containing soft-atom donor ligands, or dinuclear complexes with bridging isocyanides. The C≡N bond lengths in **5** are of interest since we observe an elongation to 1.166 Å compared to its Ni(II) analogue **4**. In addition, Ni(I) complexes tend to prefer low-coordination environments due to their electron rich nature. In fact, there are only a handful of

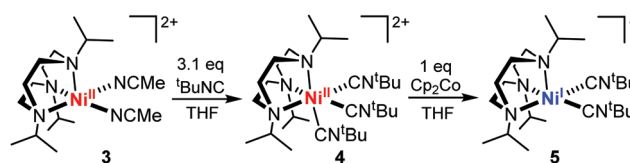


Fig. 2 Synthetic scheme for [(iPr₃TACN)Ni(I)(CN^tBu)₂](PF₆) (**5**).

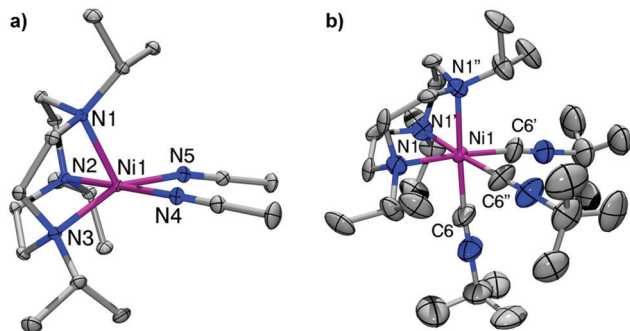


Fig. 3 ORTEP representation of the (a) solid-state structure of the cation of **3** with 50% probability ellipsoids. Selected bond lengths (Å): Ni1–N1 2.057(10); Ni1–N2 2.086(10); Ni1–N3 2.073(10); Ni1–N4 2.057(10); Ni1–N5 2.043(10); (b) Solid-state structure of the cation of **4** with 50% probability ellipsoids. Selected bond lengths (Å): Ni1–N1, 2.125(5); Ni1–C6, 1.946(8); C6–N2, 1.112(12) Hydrogen atoms, non-coordinated solvent molecules, and anions omitted for clarity.

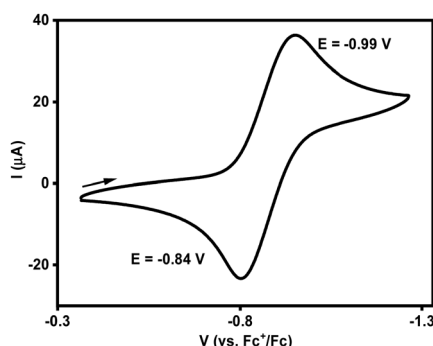


Fig. 4 CV of **4** in 0.1 M *n*-Bu₄NPF₆/MeCN (100 mV s⁻¹ scan rate).

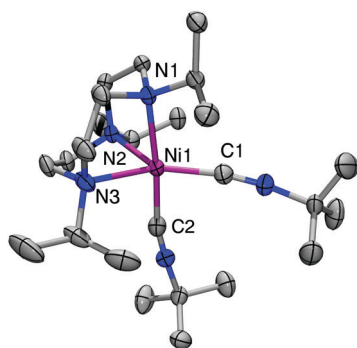


Fig. 5 ORTEP representation of the solid-state structure of the cation of **5** with 50% probability ellipsoids. Hydrogen atoms and anions omitted for clarity. Selected bond lengths (Å): Ni1–N1, 2.2044(19); Ni1–N2, 2.195(2); Ni1–N3, 2.198(2); Ni1–C1, 1.854(3); Ni1–C2, 1.933(3); C1–N4, 1.166(4); C2–N5, 1.151(3).

high-coordinate Ni(I) complexes and fewer containing redox innocent N-based ligands.⁵ To the best of our knowledge, this 5-coordinate complex is the first isolated Ni(I) complex supported by a N-based, redox innocent, TACN ligand framework.

Furthermore, the characteristic C≡N bond stretches for the Ni-bound ^tBuNC species were observed by IR. For the Ni(I) complex **5** a main stretch of $\nu_{\text{C}\equiv\text{N}} = 2165 \text{ cm}^{-1}$ was observed, within the range of reported Ni–CNR vibrational frequencies.^{40–42} Importantly, for the Ni(II) complex **4**, a higher main energy stretch of $\nu_{\text{C}\equiv\text{N}} = 2207 \text{ cm}^{-1}$ was observed. These results are expected as the more electron rich Ni(I) is likely to π -backbond to the ^tBuNC to a greater extent, which leads to the shift of the $\nu_{\text{C}\equiv\text{N}}$ stretch to lower energy.⁴³

EPR studies of **5** in a 1 : 3 MeCN:PrCN glass 77 K display a rhombic signal, consistent with a d⁹ Ni(I) center (Fig. 6a). The simulated spectrum employed *g* values of $g_x = 2.171$, $g_y = 2.121$, and $g_z = 2.018$, a superhyperfine coupling constant of 11 G in the *g_z* direction to from one N (*I* = 1) atom from the iPr₃TACN ligand. Notably, the Density Functional Theory (DFT)-calculated *g* values of 2.044, 2.198, and 2.264 agree well with the experimental EPR values. In addition, the DFT-calculated spin density was also consistent with a Ni-based unpaired electron distributed between the d_{z²} and d_{x²-y²} atomic orbitals (Fig. 6b). Bulk analysis of **5** in solution *via* the Evans method reveals a magnetic moment $\mu_{\text{eff}} = 1.68 \mu_{\text{B}}$, confirming the presence of one unpaired electron. We suspect that the bulky iPr₃TACN ligand enforces a distortion in **5**, which leads to an elongation of the Ni–N bonds and a weaker interaction between the axial nitrogen atom and the Ni(I) center. In fact, a closer look at the metrical parameters of **5** reveals a slight bend of Ni(I)–C≡NR bond angles to an average value of 169.2°, likely due to the steric clash between ^tBuNC and the isopropyl N-substituents. A similar effect was observed by Hillhouse *et al.* for the Ni(I) metal center [(IPr)Ni(CN^tBu)₃][B(Ar^F)₄] supported by a sterically encumbering N-heterocyclic carbene ligand and three distorted ^tBuNC ligands that exhibited an average Ni(I)–C≡NR bond angle of 171.2°.⁴⁴

As a direct comparison to the iPr₃TACN-supported complexes described above, we decided to synthesize the analogous Me₃TACN derivatives. Using the same synthetic method as for **5** (Fig. 3), we have employed the [(Me₃TACN)Ni(II)(MeCN)₃](BF₄)₂ complex³⁸ as a suspension in THF and added 3 equiv. of ^tBuNC, to obtain the putative [(Me₃TACN)Ni(II)(CN^tBu)₃](BF₄)₂ as a pale green solid in 90% yield. The *in situ* reduction of [(Me₃TACN)Ni(II)(CN^tBu)₃](BF₄)₂ with 1 equiv. of cobaltocene in a 1 : 3

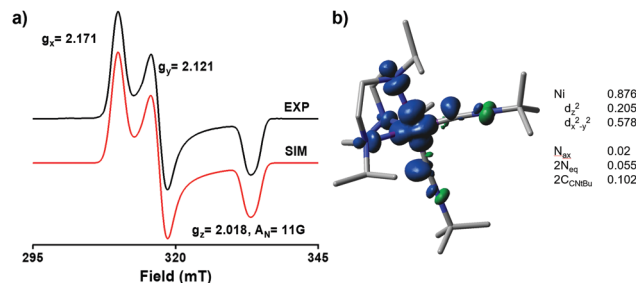


Fig. 6 (a) Experimental (1 : 3 MeCN:PrCN glass, 77 K) and simulated EPR spectra of **5**. The following parameters were used for simulation: $g_x = 2.171$; $g_y = 2.121$; $g_z = 2.018$ ($A_N = 11.0 \text{ G}$). (b) DFT-calculated Mulliken spin density for **5** (shown at a 0.002 isodensity contour plot).

THF:2-MeTHF solvent and analysis by EPR at 77 K revealed a rhombic EPR spectrum, similar to the one observed for **5**. Slightly different g values of $g_x = 2.165$, $g_y = 2.111$, and $g_z = 2.018$ were observed, along with a slightly higher superhyperfine coupling constant of 12 G from the interaction with the axial N-atom (Fig. S15, ESI[†]). The slightly higher coupling constant is in line with a decrease in steric bulk of the N-Me substituents in Me₃TACN that allow for a tighter interaction with the Ni(II) center. Notably, the [(Me₃TACN)Ni(II)(CN^tBu)₂]⁺ species was significantly less stable than **5** and could not be isolated due to its rapid decomposition within minutes at room temperature. On the other hand, complex **5** proved to be stable in solution, with no signs of decomposition after hours at RT. Overall, all these results highlight the key properties of the iPr₃TACN ligand, especially the importance of the appropriately bulky N-isopropyl groups and their ability to further stabilize the reactive metal species by sterically encumbering the low-valent Ni(II) center.

In summary, a {NiNO}¹⁰ Ni-nitrosyl complex supported by the iPr₃TACN ligand was isolated in quantitative yield from *in situ* formation of a Ni(II) species and its further reaction with NO. These results suggested that iPr₃TACN should allow that stabilization of low-valent Ni species and led us to pursue the isolation of Ni(II) complexes supported by π -acceptor ligands. We have also reported the synthesis and characterization of a Ni(II) bis-solvento MeCN complex **3**, a potentially useful Ni precursor for catalytic applications. Furthermore, the presence of ^tBuNC as an ancillary ligand allowed for the isolation of a rare 5-coordinate [(iPr₃TACN)Ni(II)(CN^tBu)₂](PF₆) complex **5**, which was characterized in detail *via* X-ray crystallography, EPR, IR, UV-Vis, and DFT calculations.

Conflicts of interest

There are no conflict to declare.

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