Methods and Results Sections of a Scientific Paper
Key Components of a Scientific Paper

1. Abstract - Concise summary of motivation, procedure, preliminary results, and research plans.

2. Introduction - Motivation for research, necessary background information for reader, important previous results, preview of findings.

3. Methods and Procedures - Description of experimental or theoretical methods used or planned, methods for data acquisition and analysis. Include figures/diagrams to convey apparatus or procedures.

4. Results and Discussion – Description/discussion of preliminary results obtained; discussion of models/hypotheses to be tested. Include figures showing any preliminary data.

5. References – Include references to the relevant scientific literature.
The Experimental Procedure

The purpose of this section is to describe the experimental or theoretical techniques and methods.

Important Elements

Techniques used: Provide enough detail so that others can replicate and evaluate the experimental or theoretical arrangement used.

Methods used: Describe general procedures used in obtaining your results, with sufficient detail for others to repeat the experiment or calculation and evaluate your methods.
The Experimental Procedure

Tips and Guidelines

Be precise in describing methods, e.g., give exact temperature values, measurement currents and voltages, etc.

You may not be able to use trade names (can be construed as advertising), unless this detail is critical to the method.

Provide any references that might help the reader understand or repeat your methods.

Don’t introduce discussion, results, or conclusions in this section.

Diagrams or figures of the experimental set-up or key parts of the apparatus are often useful—show scale and point out important features.

Describe any methods used to extract or analyze the data.
Tips and Guidelines

It has been conventional to write this section in the third-person, active-voice, past tense to emphasize the measurement (rather than the person making the measurement) and to convey what was actually done:

“X-ray diffraction measurements were performed…”

However, it is becoming more common to write in the first person, past tense to emphasize what was done and the ‘permanence’ of the result:

“We performed X-ray diffraction measurements …”
Measurement of the Damping of the Nuclear Shell Effect in the Doubly Magic $^{208}$Pb Region


The experiment was performed at the Mumbai Pelletron Linac Facility using a 30 MeV pulsed $^7$Li beam of width $\sim$1.5 ns (FWHM) and period $\sim$107 ns. Self-supporting foils of 4.7 mg/cm$^2$ $^{205}$Tl (enriched to $\geq$99%) and 3.7 mg/cm$^2$ $^{181}$Ta ($\sim$100% natural abundance) were used as targets. Alpha particles were detected at backward angles ($\sim$126°–150°) in 8 CsI(Tl) detectors of dimensions 2.5 cm × 2.5 cm × 1 cm (thick) coupled to Si(P-I-N) photodiodes and placed at a distance of $\sim$5 cm from the target. The detectors were covered with an aluminized mylar foil of thickness $\sim$1 μm. Particle identification was done using the standard pulse shape discrimination method by measuring the zero crossover timing (ZCT) of the amplified bipolar pulse.

Neutrons were detected using an array of 15 plastic detectors each of dimension 6 cm × 6 cm × 100 cm viewed by two photomultipliers, one at each end [15]. The array was placed at a mean angle of 90° to the beam direction and at a distance of 1 m from the target. The neutron energy was measured using the time of flight (TOF) technique. The data were collected in an event by event mode using a CAMAC based data acquisition system. The parameters recorded were (a) left and right timing of each plastic detector with respect to rf from the beam pulsing system using time to digital converters, (b) integrated charge of anode pulses (which is related to the electron equivalent energy, $E_{ee}$, deposited in the plastic detector) from the left and right photomultipliers using charge to digital converters, (c) timing of CsI(Tl) detectors with respect to the pulsed beam, (d) energy deposited in the CsI(Tl) detectors ($E_{cd}$), and (e) ZCT of the CsI detectors.

Third person, past tense

Notice the detail in the descriptions!
First person, present tense is becoming more common!
Effects of Particle Shape on Growth Dynamics at Edges of Evaporating Drops of Colloidal Suspensions

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Dependent capillary interactions and also varying the microscopic rules of deposition. The substantial shape fluctuations of the growth line of spheres are readily explained via a Poisson-like deposition process; slightly anisotropic particles exhibit weaker fluctuations characteristic of KPZ class behavior, and very anisotropic ellipsoids exhibit behavior consistent with the KPZ class in the presence of quenched disorder [20–22].

Our experiments employ water drops containing a suspension of polystyrene spheres (Invitrogen) stretched asymmetrically to different aspect ratios [19,23,24]. All ellipsoids are stretched from the same 1.3 μm diameter spheres; suspensions are thoroughly washed [19]. We evaporate ~μl drops centered on glass slides (Fisher Scientific) and study suspensions but with different major-minor diameter aspect ratio (ε), including spheres (ε = 1.0), slightly anisotropic particles (ε = 1.05, 1.1, 1.2), and ellipsoids (ε = 1.5, 2.5, 3.5) [25].

The experiments are reproducible across many droplets (4–10 for each aspect ratio), enabling accumulation of sufficient statistics to test continuum equation predictions of surface roughness scaling, and more. Strong shape-based capillary attractions between particles on the air-water interface [26–32] permit us to establish relationships between particle interaction and interfacial growth processes.
Nuclear Quantum Effects and Nonlocal Exchange-Correlation Functionals
Applied to Liquid Hydrogen at High Pressure

Miguel A. Morales,¹,* Jeffrey M. McMahon,² Carlo Pierleoni,³ and David M. Ceperley²

In this Letter, we present results from FP simulations based on PIMD to treat NQEs, but using nonlocal DFs in DFT. These calculations remove one of the most significant approximations made in a number of previous simulations (classical protons), while at the same time improve over another equally important and heretofore less-considered approximation (local or semilocal DFs). Such calculations allow us to study molecular dissociation in hydrogen with previously unattainable accuracy.

Simulations were performed via DFT, and we focused on two nonlocal DFs. We first chose to use the Heyd–Scuseria–Ernzerhof (HSE) DF [32], which is known to have a very small self-interaction error [33]. We also performed simulations with the second version of the van der Waals density functional (vdW-DF2) [34–37], which provides a reasonable description to exchange (for a semilocal functional), but moreover provides an improved description of nonlocal correlation (dispersion interactions) in DFT. Simulations with the former were performed with VASP [38] and the latter with a modified version of Quantum ESPRESSO (QE) [39]. A time step of 8 a.u.⁻¹ was used in all simulations, and the path integrals were discretized with a Trotter time step no larger than 0.000125 K⁻¹. After an equilibration period of ∼0.25 ps, statistics were gathered for simulation times of ∼1.5–2.0 ps, corresponding to ∼6500–9000 time steps. A Troullier-Martins norm conserving pseudopotential [40] with a core radius of $r_c = 0.5$ a.u. was used to replace the bare Coulomb potential of hydrogen in the QE simulations; a projector augmented wave method [41] was used in VASP. System sizes ranged from 128–432 atoms (a large number of atoms has been previously shown to be required for the proper description of the dissociation transition in liquid hydrogen at lower temperatures [21]). All simulations were performed at the Gamma point. The simulations with QE were performed with a plane-wave cutoff of 1224 eV, while the simulations with VASP were performed with a plane-wave cutoff of 250 eV and “accurate” settings. Finite-temperature effects on the electrons were taken into account by using Fermi–Dirac smearing [38]. While most
Observation of Spin Correlation in $t\bar{t}$ Events from $pp$ Collisions at $\sqrt{s} = 7$ TeV Using the ATLAS Detector

Beyond the SM predict different spin correlations while keeping the $t\bar{t}$ production cross section within experimental and theoretical bounds [14–18]. For example, the spin correlation measured in this Letter may differ from the SM if the $t\bar{t}$ pairs were produced via the exchange of a virtual heavy scalar Higgs boson [19] or if the top quark decayed into a scalar charged Higgs boson and a $b$ quark ($t \rightarrow H^+ b$) [20].

At the LHC $t\bar{t}$ production occurs mostly through the $gg \rightarrow t\bar{t}$ channel. At low $t\bar{t}$ invariant mass it is dominated by the fusion of like-helicity gluon pairs which produce top quarks in the left-left or right-right helicity configurations [13]. When these decay via $t\bar{t} \rightarrow W^+ W^- b\bar{b} \rightarrow l^+ \nu l^- \bar{v} b\bar{b}$ they produce charged leptons which possess correlations in azimuthal angle, $\Delta \phi$ [21], in the laboratory frame [13]. In contrast, at the Tevatron production via $q\bar{q}$ annihilation dominates. The different production mechanisms and center-of-mass energies make a measurement of the spin correlation at both colliders complementary [22]. Both the CDF and D0 Collaborations have performed measurements of the spin correlation [23–25], with a recent analysis by the D0 Collaboration reporting evidence for the presence of spin correlation in $t\bar{t}$ events with a significance of 3.1 standard deviations [26].
In this Letter, we present results from FP simulations based on PIMD to treat NQEEs, but using nonlocal DFs in DFT. These calculations remove one of the most significant approximations made in a number of previous simulations (classical protons), while at the same time improve over another equally important and heretofore less-considered approximation (local or semilocal DFs). Such calculations allow us to study molecular dissociation in hydrogen with previously unattainable accuracy.

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The Results Section

The purpose of this section is to objectively present your findings. Generally, it’s a good idea to make this section a completely objective report of your results, and to save any interpretation and comparison with working hypotheses for a separate Discussion Section.

Important Elements

Summary of results: Describe the key results obtained, with accompanying figures and graphs of raw results.

Analyzed data: Present any “converted” data obtained from an analysis of the raw data. Make sure to describe what conversion procedure was used.

Relevant details: Highlight for the reader any noteworthy observations.
The Results Section (cont.)

Tips and Guidelines

Try not to interpret, or draw conclusions from, your results in this section: Strive for a clear separation between your (presumably correct) results/calculations and your interpretations (discussion) of those results, which not everyone may agree with.

Describe things that were done in the past tense, but refer to “facts” in the present tense.

Present your results in some logical order designed to support your key conclusions (chronological order is generally not the best way). Usually it’s best to start with figures and tell a story about your research.

Present your results as clearly and concisely as possible.
Full Electric Control of Exchange Bias

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(Received 31 August 2012; published 4 February 2013)

We report the creation of a multiferroic field effect device with a BiFeO₃ (BFO) (antiferromagnetic
ferroelectric) gate dielectric and a La₀.₇Sr₀.₃MnO₃ (LSMO) (ferromagnetic) conducting channel that
exhibits direct, bipolar electrical control of exchange bias. We show that exchange bias is reversibly
switched between two stable states with opposite exchange bias polarities upon ferroelectric poling of the
BFO. No field cooling, temperature cycling, or additional applied magnetic or electric field beyond the
initial BFO polarization is needed for this bipolar modulation effect. Based on these results and the current
understanding of exchange bias, we propose a model to explain the control of exchange bias. In this model
the coupled antiferromagnetic-ferroelectric order in BFO along with the modulation of interfacial
exchange interactions due to ionic displacement of Fe³⁺ in BFO relative to Mn³⁺/⁴⁺ in LSMO cause bipolar modulation.

DOI: 10.1103/PhysRevLett.110.067202

PACS numbers: 85.70.Kh, 75.30.Et, 75.47.Lx
To investigate the magnetic properties of the LSMO channel, we measured its electrical resistance as a function of applied in-plane magnetic field in both the [100] ($B_x$) and [010] ($B_y$) directions, separately, as depicted in Figs. 1(a) and 1(b). Each magnetotransport measurement is performed at a static temperature, and at no point in the experiment was the device cooled in any electric or magnetic field. Typical measurements for both BFO FE polarizations are shown in Fig. S1 of the Supplemental Material [11]. The data exhibit magnetic hysteresis and have coercive and saturation features analogous to that of an $M$-$H$ hysteresis loop. We interpret the peaks in resistance as the coercive fields where there is zero net magnetization and that the tail is where magnetization becomes saturated. By determining these peak positions we determine the magnetic coercivity (distance between the peaks) and exchange bias (shift in the peaks off the origin) as shown in Fig. S1 [11]. Results using this technique are in excellent agreement with SQUID magnetometer $M$-$H$ measurements on unpatterned films and are further detailed in our previous work on such devices [9].

To examine the effect of BFO polarization on exchange bias, a ±24 V voltage pulse was applied between the gate and the LSMO channel to polarize the BFO in the [001] direction. Measurements show that BFO polarization out of plane is fully saturated; however, complex domain structures may still form in plane since there are still four degenerate in-plane polarization states [9]. These structures are difficult to observe in our device due to the Au top electrode, but we can draw parallels from piezoresponse-force microscopy images for unpatterned BFO-LSMO heterostructures from previous work [9]. Magnetoresistance is measured and exchange bias is then
Notice how the authors are just telling a story about their figure and stating the facts of their data.

FIG. 2 (color online). (a) Gate pulse sequence applied before carrying out magnetoresistance measurements (green, left arrow) and the corresponding sheet resistance of the LSMO (purple, right arrow). (b), (c) Measurements of exchange bias and coercivity taken at 5.5 K after gate pulse shown in (a). Panels (b) and (c) represent the data when voltage pulses are applied in positive and negative remanent magnetization, respectively. Current was applied along the [110] direction with applied magnetic field in the $B_x$ [100] direction.

PRL 110, 067202 (2013) PHYSICAL REVIEW LETTERS

on three separate epitaxially grown heterostructures. Figures 2(b) and 2(c) show bipolar modulation with respect to gate pulse at 5.5 K in both remanent magnetization states for a device patterned along the [110] (Fig. 1(b)) direction with a magnetic field applied in [100] ($B_x$). Depending on the remanent magnetization state of LSMO upon application of gate pulses, opposite FE polarizations lead to opposite directions of exchange bias. The modulation behavior is mirrored through the zero exchange bias axis between different remanent magnetization states. The temperature of the sample was held at 5.5 K throughout the measurement. The sole determining factors for the polarity of exchange bias in these bipolar devices are (a) the polarization state of the BFO film and (b) the $M_R$ of LSMO. To offer a comparison of the bipolar modulation behavior to unipolar modulation, a plot is presented in the supplemental figure Fig. S2 [11].
The authors characterize their results, but they do not interpret what the results mean in this section.

Again, they’re telling a story about their figure…this is why it helps to generate your figures first!
The Discussion Section

The goal of this section is to provide an interpretation of your results, support for your conclusions, and a comparison of your results to relevant hypotheses.

Important Elements

**Detailed Analysis:** Analyze your results with an appropriate level of detail. Compare your results with previous results.

**Hypothesis testing:** If your results agree or differ with particular models, provide an explanation of the relevant hypotheses, and explain in detail why you believe your results agree or disagree with these models.
Modulation disappears around 30 K, well below the blocking temperature of this system which was previously determined to be around 100–120 K.

We can now speculate on the mechanism behind the electric field control of exchange bias in this system. The most recent exchange bias models are based on the existence of an interface state between the AFM and FM that is markedly different than either the FM or the AFM individually [12]. Such an interface state will produce two different types of spins that contribute unequally to the exchange bias system [13–16]. Some interface spins will become pinned in a single direction by the AFM, unaffected by magnetic field. The interaction between these pinned spins and the FM causes an effective “bias field” that the underlying FM layer must overcome before magnetization can be switched, resulting in exchange bias. Other interface spins will rotate with the FM layer when the magnetic field is swept, because they are coupled more tightly to the FM than the AFM. This results in a spin drag effect that increases the coercivity of the FM material. Several groups have observed these types of magnetic interface interactions [5,6]. Previous work showed an emergent interfacial magnetic state, correlated with exchange bias, in BFO-LSMO heterostructures resulting from the enhanced canting of the AFM spins at an otherwise magnetically compensated interface [17]. Furthermore, in this system the coupling between Fe$^{3+}$ in the magnetic interface layer and the Mn$^{3+/4+}$ was antiferromagnetic. Many exchange bias systems exhibit this type of AFM interfacial coupling, but no differences in exchange bias occur until extremely high magnetic fields are applied to overcome the interfacial coupling and align all spins to the external magnetic field. Since we do not use such high fields, the exchange bias model described above does not change. Some spins will be pinned, and some will rotate with the FM; since the coupling to the interface layer is antiferromagnetic, the interface spins will evolve in the opposite fashion as compared to the ferromagnetically coupled case [18].
Comparison with models

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The Discussion Section

Comparison with previous data
Interpretation of results

The Discussion Section

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Based on these models we present an explanation for the following effects: bipolar exchange bias modulation, the remanent magnetization dependence of that modulation, and coercivity modulation. The progression of the magnetic state in our device as magnetic field is swept and after a gate pulse reverses BFO polarization is shown in Fig. 4. Figure 4(a) shows the progression in terms of a magnetic hysteresis loop and Fig. 4(b) shows it from an interfacial spin state perspective. Because of the ferroelectric nature of BFO, when ferroelectric polarization is switched, the Fe and Bi ions will move relative to the oxygen octahedra [19]. Since the LSMO channel does not exhibit the same effect, the Fe ion at the interface in BFO exists in two different states depending on FE polarization, one closer to the LSMO channel and one farther away. The AFM anisotropy is much greater than the FM anisotropy [20,21];
Nuclear Quantum Effects and Nonlocal Exchange-Correlation Functionals
Applied to Liquid Hydrogen at High Pressure

Miguel A. Morales,\textsuperscript{1,*} Jeffrey M. McMahon,\textsuperscript{2} Carlo Pierleoni,\textsuperscript{3} and David M. Ceperley\textsuperscript{2}
Figure 3 shows a comparison of pressure versus density along the $T = 1000$ K isotherm for both FPMD and PIMD simulations using either PBE DFs [21] or vdw-DF2. Notice that both DFs show a plateau in the pressure, a clear indication of a first-order LLPT. There is, however, a further qualitative similarity in that the transition occurs between an insulating molecular liquid and a conductive atomiclike liquid. There is a large quantitative difference in the transition pressures. The inset of Fig. 3 shows a comparison of the PCF between FPMD and PIMD simulations using vdw-DF2. As can be seen, NQEs have a strong influence on the properties of the molecular peak, zero-point motion producing a wider distribution of bond distances. This results in a destabilization of the molecular state, explaining the lower transition pressures. (Notice that the primary vdw-DF2 results shown in the figure are performed with PIMD, so systems of classical protons are expected to exhibit even higher transition pressures, above 365 GPa).
Presentation of results; Note that you can characterize your results, just don’t interpret them here.

Figure 4 shows the electronic conductivity as a function of pressure along various isotherms, comparing both PBE and HSE DFs. Note that in both cases, proton configuration were generated with vdw-DF2. Notice also that while the conductivity values differ between HSE and PBE DFs, they nonetheless agree on the existence of a jump at $T = 1000$ K.

Returning to Fig. 1, a schematic phase diagram of hydrogen in the regime of molecular dissociation and below...
Comparison with previous results

$T = 6000 \text{ K}$ can be seen. The previously reported LLPT, obtained with classical protons and either from FPMD + PBE or coupled electron-ion Monte Carlo (CEIMC) [21] calculations are shown [49]. Both vdw-DF2 (present work) and CEIMC calculations show a considerable increase in the transition pressures with respect to PBE DFs, with those from vdw-DF2 being considerably higher. Above the critical point, state points of an electronic conductivity of $\sigma = 2000 \text{ (}\Omega\text{ cm)}^{-1}$, separating the insulating from metallic liquid [50], are also reported using either vdw-DF2 or PBE. Loubeyre et al. [47] reported that the metal-to-insulating threshold was located at conditions of 10% reflectivity, since according to the Drude model, this corresponds to an ionization of 1%. The present criterion for metallic behavior is different though. For example, from our reflectivity data, a minimum metallic conductivity of $\sigma = 2000 \text{ (}\Omega\text{ cm)}^{-1}$ corresponds to a reflectivity of $\sim 0.35 - 0.40$ which is closer to 70% of its saturation value ($\sim 0.6$). This explains why our threshold line is in apparent disagreement with the experimental points reported in Ref. [47]. In fact, at conditions of 10% reflectivity, close to the precompressed-state Hugoniot curve, we observe conductivities on the order of $\sigma = 100 - 500 \text{ (}\Omega\text{ cm)}^{-1}$. Figure 1 also shows the result from the reverberation shock compression of S. Weir et al. [50]. While the temperature was not measured therein experimentally, but rather estimated using a model EOS, and the error bars were rather large, it is nonetheless clear that the presented results of the location of the LLPT and the dissociation regime at higher temperatures agree rather well.

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The Discussion Section
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While almost all FP simulation methods agree qualitatively on the existence of a first-order LLPT in high-pressure hydrogen [21,23], its precise location depends on the approximations employed. The results reported above clearly show that NQEs and nonlocal DFs in DFT play an important role in the description of molecular dissociation and metallization. The two DFs considered (HSE and vdW-DF2) were originally developed with the goal of addressing significant limitations of local and semilocal DFs in DFT. HSE, on the one hand, was developed to reduce self-interaction errors in PBE in its applications to solids [32]. Such errors lead to a strong tendency to favor delocalized electronic states, which in turn lead to an underestimation of band gaps by as much as 1–2 eV (in hydrogen) [24]. This leads to a serious underestimation of the metallization pressures in both liquid and solid phases, and a tendency to favor metallic states (e.g., solid structures). vdW-DF and its improved version vdW-DF2 (employed in this work), on the other hand, were developed to account for nonlocal electron correlations, such as dispersion interactions in DFT. The presented results indicate that, at least close to dissociation, both HSE and vdW-DF2 DFs produce very similar structures in liquid hydrogen. Since the physical effects addressed by both DFs are not directly related to each other, and that both effects are expected to be relevant in the molecular phase, it is important to recognize that the LLPT pressures might still
Discussion of different interpretations

change if a DF which combines both hybrid exchange and nonlocal correlation were to be employed.

The goal of this Letter was not to predict which functional (HSE or vdW-DF2, etc.) is more accurate, since answering that question requires the use of more accurate methods [51]. We can however mention several possibilities that explain the observed behavior, the reasonable agreement between either nonlocal DF as well as their large disagreements with PBE DFs. Both DFs predict shorter molecular bonds compared to PBE; in the limit of low density, the bond length predicted by vdW-DF2 agrees very well with measured values while that of PBE DFs is overestimated by \( \sim 3\% \) [52]. This is obviously an important factor on dissociation. Second, the exchange portion of the vdW-DF2 functional was constructed to reproduce exact-exchange results [37], which may explain its similarity to HSE. Finally, both dispersion interactions and a reduced self-interaction will lead to a more stable molecular state. An even more promising alternative to DFT is the use of quantum Monte Carlo first-principles methods, for example CEIMC [21], using accurate trial wave functions, such as those constructed from HSE orbitals. We must also recognize that, while the use of the vdW-DF2 DF made large improvements in the description of molecular dissociation in hydrogen near the LLPT, standard semilocal DFs like PBE have been shown to be successful in describing other materials when combined with the HSE DF for the calculation of optical properties [53].