

Mon. April 17, 2017 – David Harrison, WFU (Ph. D. Thesis; Mentor: T. Thonhauser) Improving Existing and Discovering New Hydrogen Storage Materials Using Computational Materials Modeling Note: Public talk will begin at 12:30 PM in ZSR 204.
Mon. April 17, 2017 – Ryan Godwin, WFU (Ph. D. Thesis; Mentor: F. Salsbury) Binding NEMO: Adventures in Molecular Dynamics Note: Public talk will begin at 3:00 PM in Cfm 101.
Wed. April 19, 2017 – Honors presentations Part I –
Fri. April 21, 2017 – Larry Rush, WFU (MS. Thesis; Mentor: N. Holzwarth) Note: Public talk will begin at 12:30 PM in Scales 009.
Mon. April 24, 2017 – Xiaohua (Nina) Liu, WFU (Ph. D. Thesis; Mentor: D. Kim-Shapiro) "Effects of Red Blood Cells on Nitric Oxide Bioactivity" Note: Public talk will begin at 10:00 AM in ZSR 204.
Wed. Apr. 26, 2017 – Honors presentations Part II –
Thur. April 27, 2017 – Crystal Bolden, WFU (Ph. D. Thesis; Mentor: D. Kim-Shapiro) "Interaction between RSNO and H₂S: The formation, stability, and NO-donating capacity of SSNO" and the effects of SSNO" on platelet activation" Note: Public talk will begin at 9:00 AM in ??

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Definition of a linear Lie group

1. A linear Lie group is a group
 - Each element of the group T forms a member of the group T' when "multiplied" by another member of the group $T''=T \cdot T'$
 - One of the elements of the group is the identity E
 - For each element of the group T , there is a group member a group member T' such that $T \cdot T'=E$.
 - Associative property: $T \cdot (T' \cdot T'') = (T \cdot T') \cdot T''$
2. Elements of group form a "topological space"
3. Elements also constitute an "analytic manifold"

→ Non countable number elements lying in a region "near" its identity

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Definition: Linear Lie group of dimension n

A group G is a linear Lie group of dimension n if it satisfied the following four conditions:

1. G must have at least one faithful finite-dimensional representation Γ which defines the notion of distance.

For represent Γ having dimension m , the distance between two group elements T and T' can be defined:

$$d(T, T') \equiv \left\{ \sum_{j=1}^m \sum_{k=1}^m \left[\Gamma(T)_{jk} - \Gamma(T')_{jk} \right]^2 \right\}^{1/2}$$

Note that $d(T, T')$ has the following properties

- (i) $d(T, T') = d(T', T)$
- (ii) $d(T, T) = 0$
- (iii) $d(T, T') > 0$ if $T \neq T'$
- (iv) For elements T, T' , and T'' ,

$$d(T, T') \leq d(T, T'') + d(T', T'')$$

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Definition: Linear Lie group of dimension n -- continued

2. Consider the distance between group elements T with respect to the identity E -- $d(T,E)$. It is possible to define a sphere M_δ that contains all elements T' such that $d(E,T') \leq \delta$.

It follows that there must exist a $\delta > 0$ such that every T' of G lying in the sphere M_δ can be parameterized by n real parameters x_1, x_2, \dots, x_n such each T' has a different set of parameters and for E the parameters are $x_1 = 0, x_2 = 0, \dots, x_n = 0$

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Definition: Linear Lie group of dimension n -- continued

3. There must exist $\eta > 0$ such that for every parameter set $\{x_1, x_2, \dots, x_n\}$ corresponding to T' in the sphere M_δ :

$$\sum_{j=1}^n x_j^2 < \eta^2$$

4. There is a requirement that the corresponding representation is analytic

For element T' within M_δ , $\Gamma(T'(x_1, x_2, \dots, x_n))$ must be an analytic (polynomial) function of x_1, x_2, \dots, x_n .

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Some more details

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For element T' within M_δ , $\Gamma(T'(x_1, x_2, \dots, x_n))$ must be an analytic (polynomial) function of x_1, x_2, \dots, x_n .

Because of the mapping to the n parameters x_1, x_2, \dots, x_n to each group element T' , $\Gamma(T'(x_1, x_2, \dots, x_n)) = \Gamma(x_1, x_2, \dots, x_n)$.

The analytic property of $\Gamma(x_1, x_2, \dots, x_n)$ also means that derivatives

$$\frac{\partial^\alpha \Gamma_{jk}(x_1, x_2, \dots, x_n)}{\partial x_p^\alpha}$$

must exist for all $\alpha = 1, 2, \dots$

Define $n \times m \times m$ matrices:

$$(\mathbf{a}_p)_{jk} \equiv \left. \frac{\partial \Gamma_{jk}(x_1, x_2, \dots, x_n)}{\partial x_p} \right|_{x_1=0, x_2=0, \dots, x_n=0}$$

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Definition: Real Lie algebra
 A real Lie algebra of dimension $n \geq 1$ is a real vector space of dimension n which includes a comutator $[M, N]$ as follows:

1. For all M, N in algebra, $[M, N]$ is also in algebra
2. For real numbers α and β , and members M, N, O ,
 $[\alpha M + \beta N, O] = \alpha[M, O] + \beta[N, O]$
3. $[M, N] = -[N, M]$
4. $[M, [N, O]] + [N, [O, M]] + [O, [M, N]] = 0$

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Structure constants of Lie algebra
 Consider the n basis matrices of the algebra $\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n$:

$$[\mathbf{a}_p, \mathbf{a}_q] = \sum_{r=1}^n c_{pq}^r \mathbf{a}_r \quad \text{for } p, q=1, 2 \dots n$$

Example: G is the group $SU(2)$ of all 2×2 unitary matrices having determinant 1

$$\mathbf{a}_1 = \frac{1}{2} \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} \quad \mathbf{a}_2 = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad \mathbf{a}_3 = \frac{1}{2} \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$$

Structure constants for this case:

$$[\mathbf{a}_1, \mathbf{a}_2] = -\mathbf{a}_3 \quad [\mathbf{a}_2, \mathbf{a}_3] = -\mathbf{a}_1 \quad [\mathbf{a}_3, \mathbf{a}_1] = -\mathbf{a}_2$$

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Fundamental theorem –

For every linear Lie group there exists a corresponding real Lie algebra of the same dimension. For example if the linear Lie group has dimension n and has $m \times m$ matrices $\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n$ then these matrices form a basis for the real Lie algebra.

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One-parameter subgroup of a linear Lie group

A "one-parameter subgroup" of a linear Lie group fulfills the requirements of a Lie group as a subgroup whose elements $T(t)$ depend on a real parameter t with $-\infty < t < \infty$ where

$$T(s)T(t) = T(s+t)$$

Note that $T(s)T(t) = T(t)T(s)$ so that the subgroup is Abelian. It follows that $T(t=0) = E$

Theorem: Every one-parameter subgroup of a linear Lie group of $m \times m$ matrices is formed by exponentiation of

$$m \times m \text{ matrices. } \mathbf{A}(t) = e^{t\mathbf{a}} \quad \mathbf{a} = \left. \frac{d\mathbf{A}}{dt} \right|_{t=0}$$

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$$\frac{d\mathbf{A}(t)}{dt} = \lim_{s \rightarrow 0} \left(\frac{\mathbf{A}(t+s) - \mathbf{A}(t)}{s} \right) = \lim_{s \rightarrow 0} \left(\mathbf{A}(t) \left(\frac{\mathbf{A}(s) - \mathbf{A}(0)}{s} \right) \right) = \mathbf{A}(t)\mathbf{a}$$

$$\mathbf{A}(t) = e^{t\mathbf{a}}$$

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Correspondence between each linear Lie group \mathcal{G} and a real Lie algebra \mathcal{L} Simplify the consideration to \mathcal{G} consisting of $m \times m$ matrices $\mathbf{T} = \mathbf{A}$ and $\Gamma(\mathbf{T}) = \mathbf{A}$.

As part of the definition of the linear Lie group, there are n parameters x_1, x_2, \dots, x_n such that all $\mathbf{A}(x_1, x_2, \dots, x_n)$ are analytic functions of the parameters, and the $n \times m \times m$ matrices

$$\left(\mathbf{a}_p \right)_{jk} = \left. \frac{\partial \mathbf{A}}{\partial x_p} \right|_{x_1=x_2=\dots=x_n=0}$$

form the basis of an n -dimensional real vector space.

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Definition: Analytic curve in \mathcal{G}
 Suppose $x_1(t), x_2(t), \dots, x_n(t)$ are analytic functions of $0 \leq t \leq t_0$ within which $\sum_{j=1}^n x_j^2(t) \leq \eta^2$, then the set of $m \times m$ matrices $\mathbf{A}(t) = \mathbf{A}(x_1(t), x_2(t), \dots, x_n(t))$ are said to form an analytic curve in \mathcal{G} .

Definition: Tangent vector of an analytic curve in \mathcal{G}
 The tangent vector of an analytic curve $\mathbf{A}(t)$ in \mathcal{G} is defined to be the $m \times m$ matrix $\mathbf{a} = \left. \frac{d\mathbf{A}(t)}{dt} \right|_{t=0}$.

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Theorem The tangent vector of any analytic curve in \mathcal{G} is a member of the real vector space having the matrices $\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n$ as its basis. Conversely, every member of the real vector space is the tangent vector of some analytic curve in \mathcal{G} .

Theorem If \mathbf{a} and \mathbf{b} are the tangent vectors of the analytic curves $\mathbf{A}(t)$ and $\mathbf{B}(t)$ in \mathcal{G} , then $\mathbf{c} = [\mathbf{a}, \mathbf{b}]$ is the tangent vector of the analytic curve $\mathbf{C}(t)$ in \mathcal{G} , where

$$\mathbf{C}(t) = \mathbf{A}(\sqrt{t})\mathbf{B}(\sqrt{t})(\mathbf{A}(\sqrt{t}))^{-1}(\mathbf{B}(\sqrt{t}))^{-1}$$

Note that $\mathbf{A}(\sqrt{t}) \approx 1 + \mathbf{a}\sqrt{t} + O(t)$

$$\mathbf{C}(t) \approx (1 + \mathbf{a}\sqrt{t} \dots)(1 + \mathbf{b}\sqrt{t} \dots)(1 - \mathbf{a}\sqrt{t} \dots)(1 - \mathbf{b}\sqrt{t} \dots)$$

$$\approx 1 + \mathbf{a}\mathbf{b}t - \mathbf{b}\mathbf{a}t \dots \Rightarrow \left. \frac{d\mathbf{C}(t)}{dt} \right|_{t=0} = [\mathbf{a}, \mathbf{b}]$$

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Fundamental theorem: For every linear Lie group \mathcal{G} there exists a corresponding real Lie algebra \mathcal{L} of the same dimension. More precisely, if \mathcal{G} has dimension n then the $m \times m$ matrices $\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n$ form a basis for \mathcal{L} .

Converse to fundamental theorem: Every real Lie algebra is isomorphic to the real Lie algebra of some linear Lie group.

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Example: SO(3)

In this case, it is convenient to consider rotations about the 3 orthogonal directions:

$$R(\alpha, \beta, \gamma) = R(\alpha, \hat{x})R(\beta, \hat{y})R(\gamma, \hat{z})$$

$$= \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \alpha & -\sin \alpha \\ 0 & \sin \alpha & \cos \alpha \end{pmatrix} \begin{pmatrix} \cos \beta & 0 & \sin \beta \\ 0 & 1 & 0 \\ -\sin \beta & 0 & \cos \beta \end{pmatrix} \begin{pmatrix} \cos \gamma & -\sin \gamma & 0 \\ \sin \gamma & \cos \gamma & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\left. \frac{\partial R}{\partial \alpha} \right|_{\alpha=\beta=\gamma=0} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \equiv -\mathbf{a}_1$$

$$\left. \frac{\partial R}{\partial \beta} \right|_{\alpha=\beta=\gamma=0} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} \equiv -\mathbf{a}_2$$

$$\left. \frac{\partial R}{\partial \gamma} \right|_{\alpha=\beta=\gamma=0} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \equiv -\mathbf{a}_3$$

Note that:

$$[\mathbf{a}_1, \mathbf{a}_2] = -\mathbf{a}_3$$

$$[\mathbf{a}_2, \mathbf{a}_3] = -\mathbf{a}_1$$

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