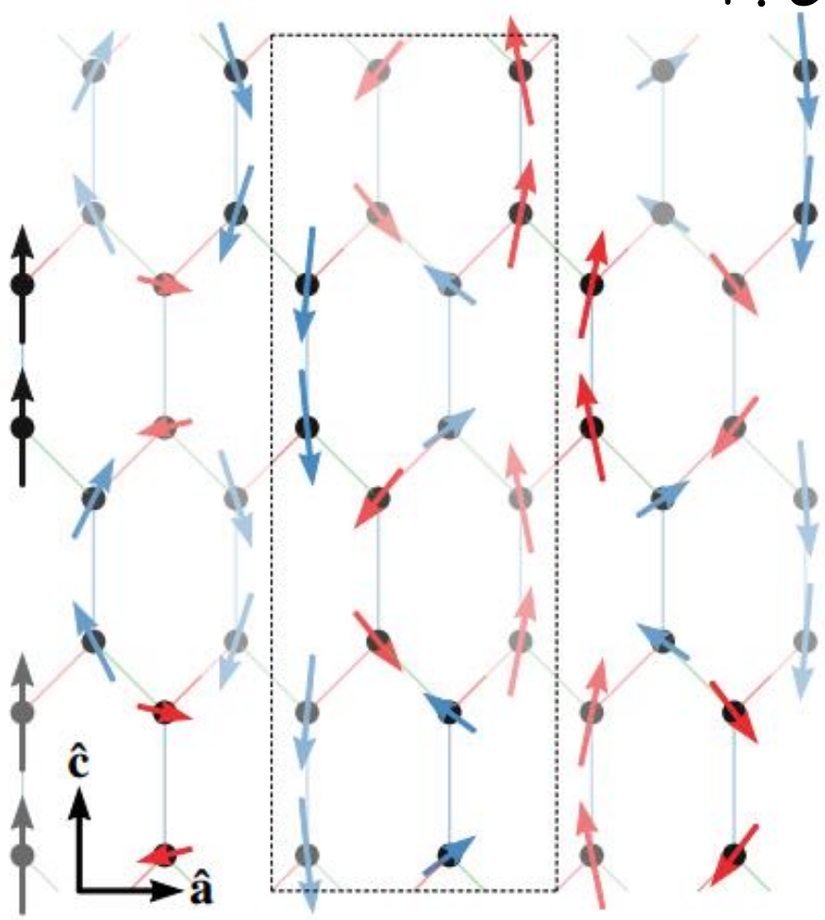
β-Li_2IrO_3

Counter-rotating Incommensurate Non-Coplanar Spiral Orders

Radu Coldea,
P. Gegenwart (2014)

EXPERIMENT



$$\mathbf{Q}_{\text{exp}} = (0.57, 0, 0)$$

$$(iA_a, iC_b, F_c)$$

$$F = [+,+,+,+]$$
$$C = [+,+,-,-]$$
$$G = [+,-,+,-]$$
$$A = [+,-,-,+]$$

β-Li_2IrO_3

Counter-rotating Incommensurate Non-Coplanar Spiral Orders

Radu Coldea,
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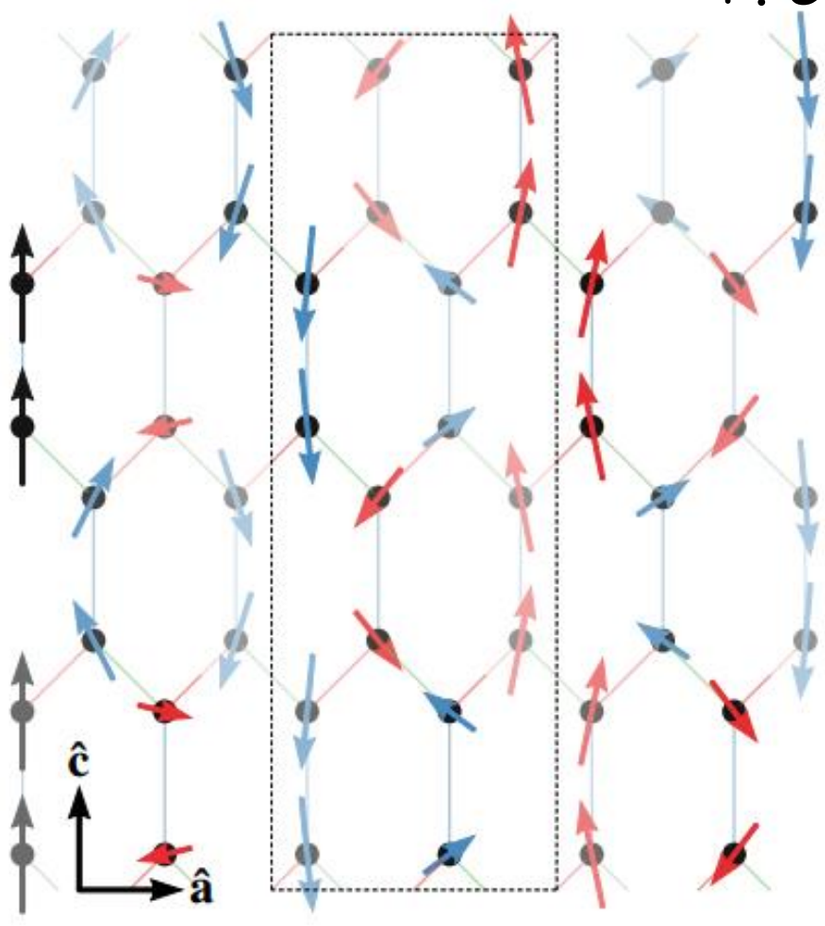
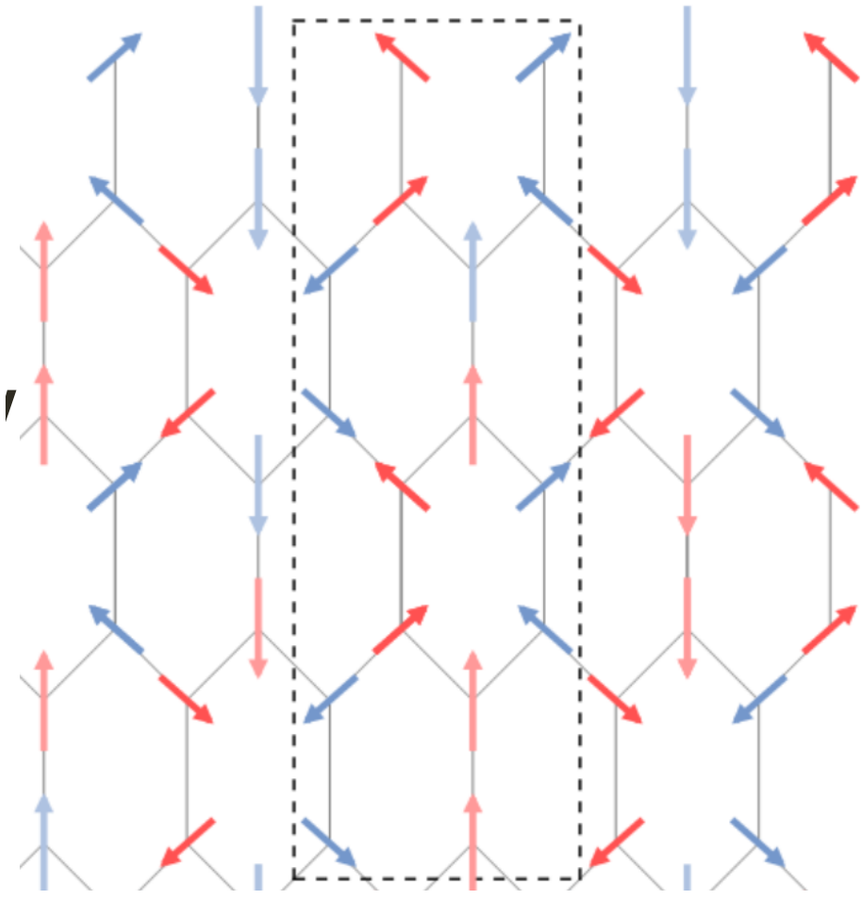


$\mathbf{Q}_{\text{exp}} = (0.57, 0, 0)$

(iA_a, iC_b, F_c)

SYMMETRY AGREES

THEORY



$\mathbf{Q} = (h'00) \;\; 0.53 \lesssim h' \lesssim 0.80$

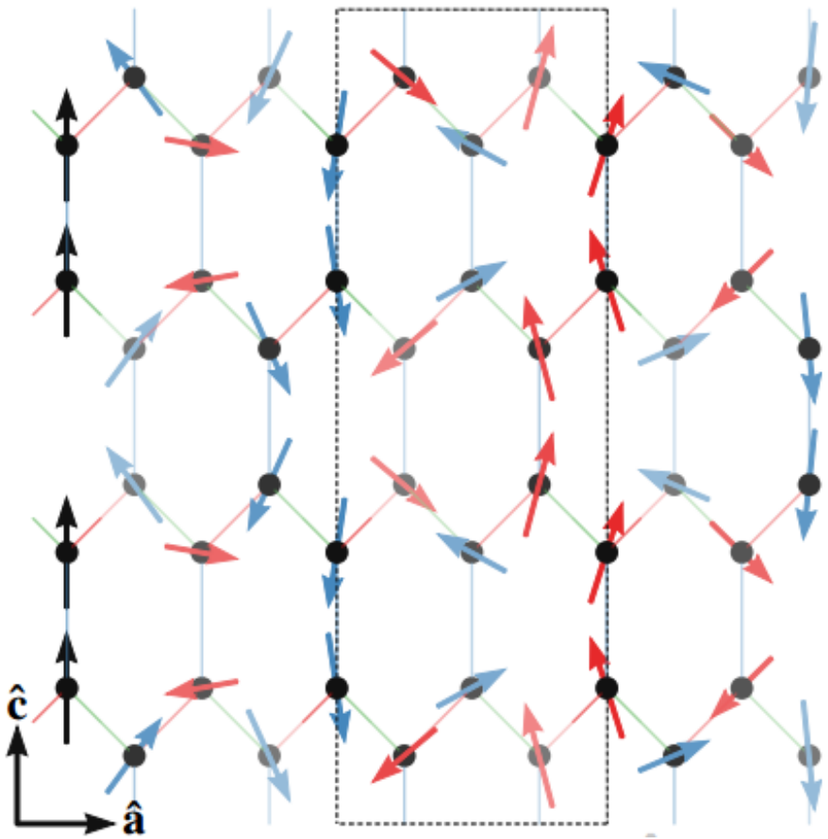
(iA_a, iC_b, F_c)

γ-Li_2IrO_3

Counter-rotating Incommensurate Non-Coplanar Spiral Orders

Radu Coldea,
James Analytis
(2014)

EXPERIMENT



$$\mathbf{Q}_{\text{exp}} = (0.57, 0, 0)$$

$$[i(A,-A)_a, (-1)^m i(F,-F)_b, (\bar{F},F)_c]$$

$$F = [+,+,+,+]$$
$$C = [+,+,-,-]$$
$$G = [+,-,+,-]$$
$$A = [+,-,-,+]$$

γ-Li_2IrO_3

Counter-rotating Incommensurate Non-Coplanar Spiral Orders

Radu Coldea,
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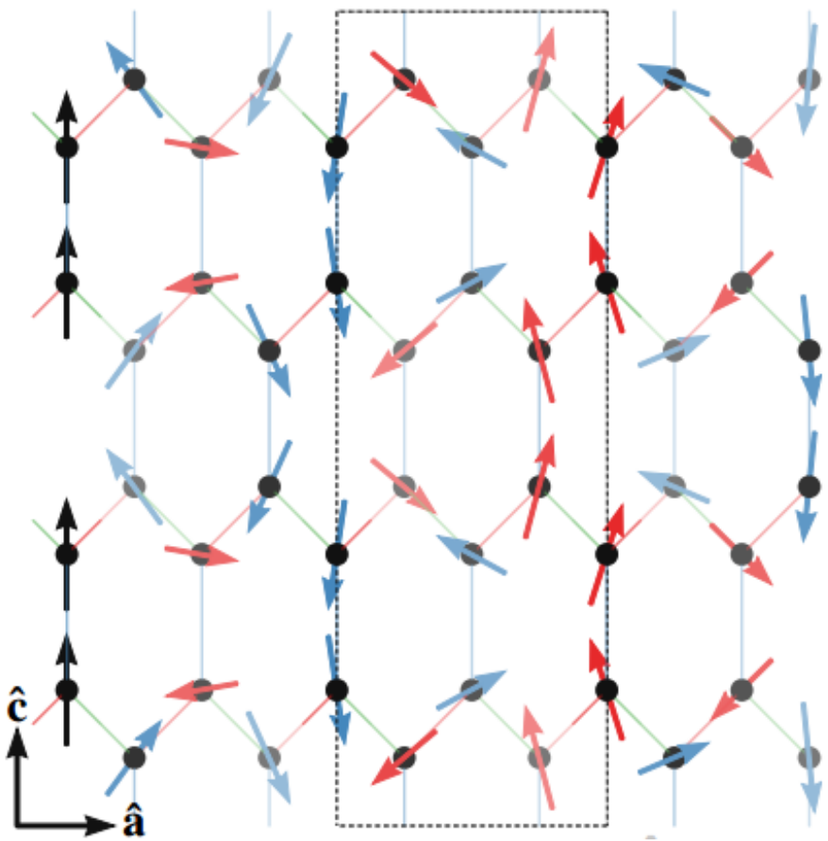
(2014)

EXPERIMENT

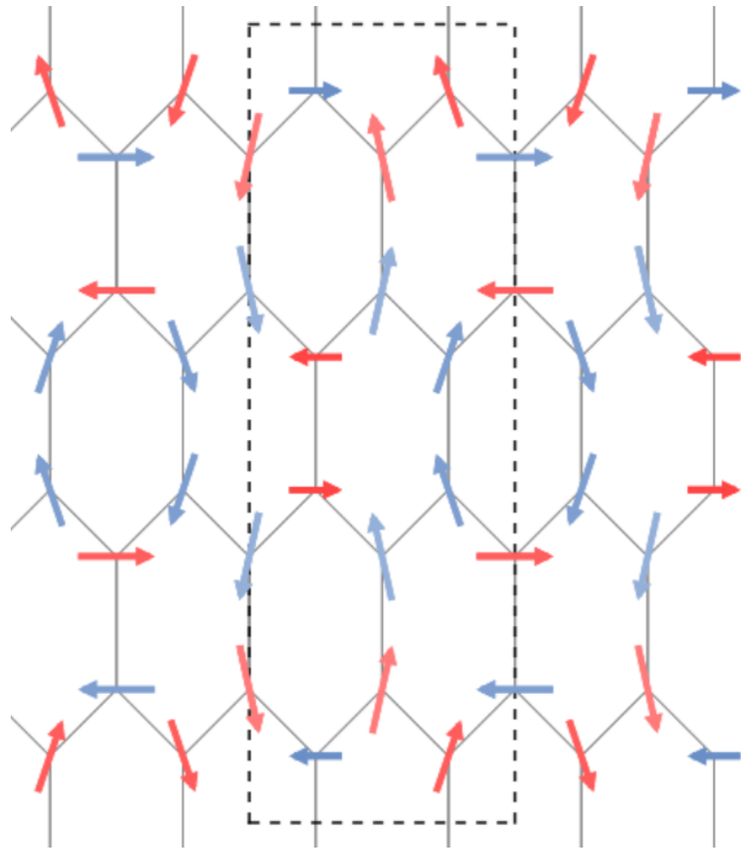


$$\mathbf{Q}_{\text{exp}} = (0.57, 0, 0)$$

$$[i(A,-A)_a, \boxed{(-1)^m i(F,-F)_b}, (\bar{F},F)_c]$$

SYMMETRY DISAGREES IN b COMP

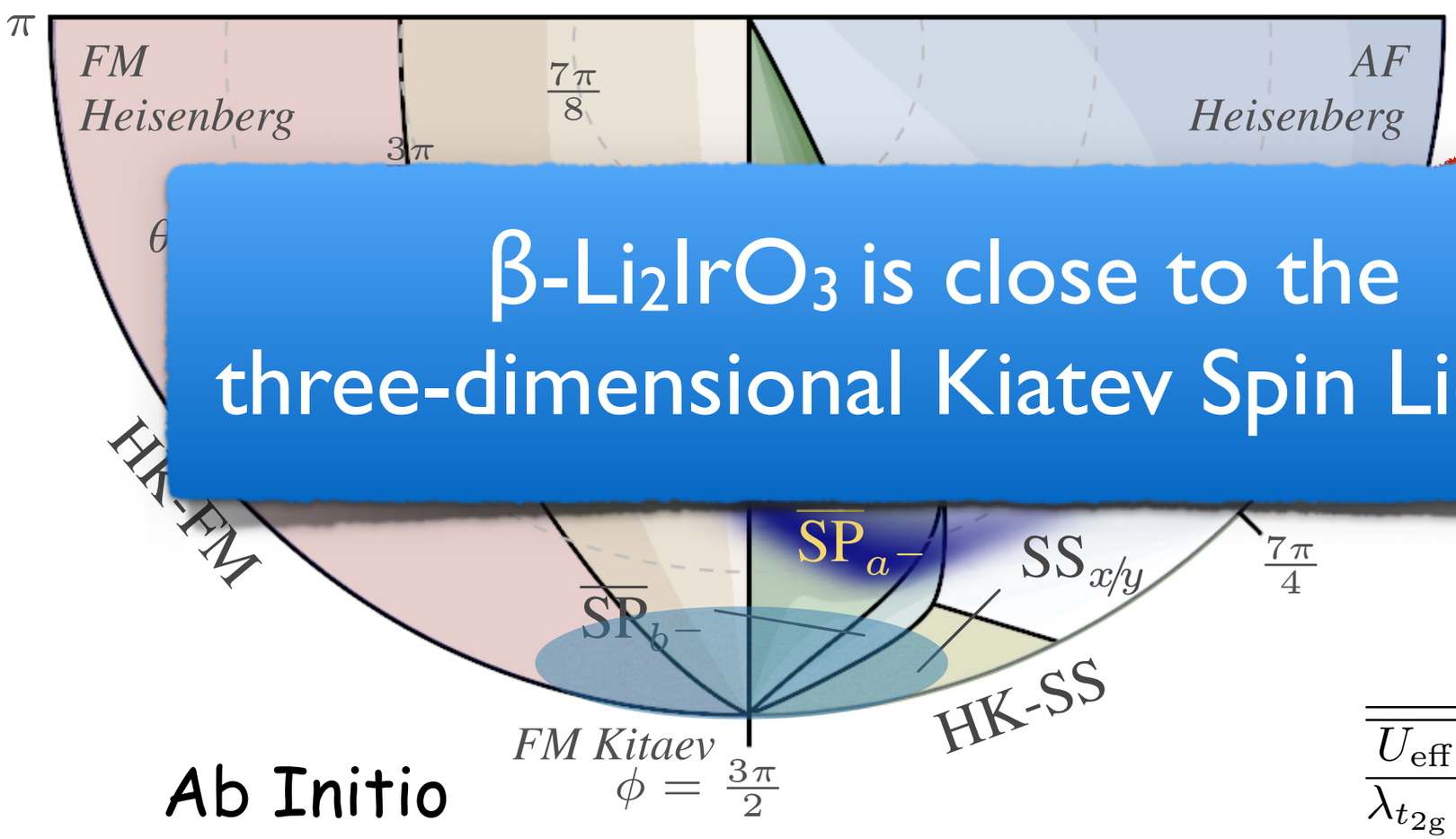
THEORY



$$\mathbf{Q} = (h'00) \quad 0.53 \lesssim h' \lesssim 0.80$$

$$[i(A,-A)_a, \boxed{-i(C,-C)_b}, (F,F)_c]$$

$$H = \sum_{\langle ij\rangle \in \alpha\beta(\gamma)} \left[J\vec{S}_i \cdot \vec{S}_j + KS_i^\gamma S_j^\gamma + \Gamma\left(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha\right)\right]$$



(iA_a, iC_b, F_c)

-rotating
ensurate
oplanar
Spiral Order

β-Li_2IrO_3 is close to the three-dimensional Kiatev Spin Liquid !

Ab Initio
(OpenMx, PBE-GGA)

For a range of values of

$U_{\text{eff}} \sim 1{-}3\ eV \qquad J_H \sim 50{-}300\ meV$

U_{eff} (eV)		0.0	1.5	3.0
$\lambda_{t_{2g}}$		0.401	0.482	0.516
t_1	Z	+0.085	+0.077	+0.064
	X	+0.083	+0.074	+0.058
$\lvert t_2\rvert$	Z	0.238	0.255	0.270
	X	0.260	0.276	0.289
t_3	Z	-0.162	-0.119	-0.060
	X	-0.153	-0.110	-0.055

Coupled Zig-Zag Chain (CZC) Model

FM KITAEV, HIGHLY BOND ANISOTROPIC

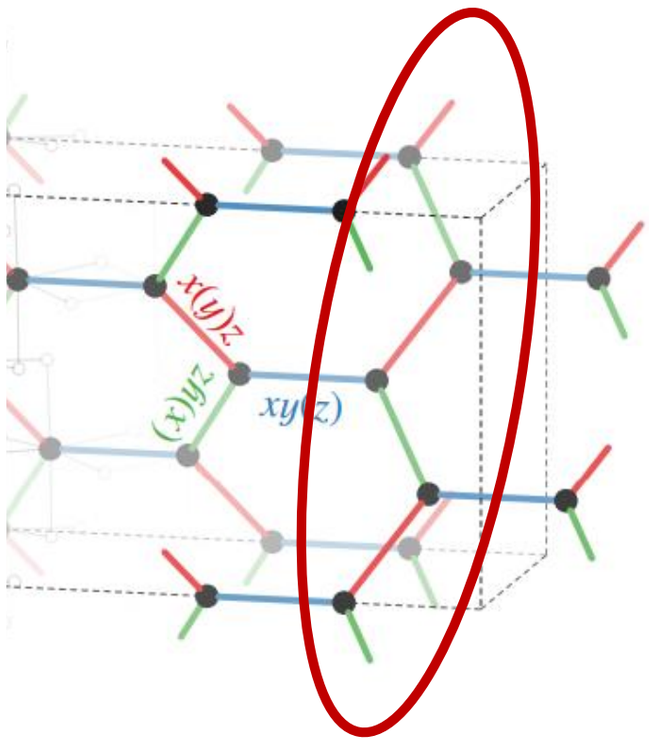
$$H = \sum_{\langle ij\rangle\in\gamma} [J\vec{S}_i\cdot\vec{S}_j + KS_i^\gamma S_j^\gamma] + \sum_{\langle ij\rangle\in Z} I_c(\hat{r}_{ij}\cdot\vec{S}_i)(\hat{r}_{ij}\cdot\vec{S}_j)$$

$$J_Z = J + \frac{1}{2}I_c \qquad K_Z = K - \frac{1}{2}I_c$$

$$J_{X/Y} = J \qquad K_{X/Y} = K$$

$$\Gamma_Z = \frac{1}{2}I_c$$

$$\Gamma_{X/Y} = 0$$



I KIMCHI, R COLDEA, A VISHWANATH
PRB 91, 245134 (2015)

Comparison Study

MODELS

JKΓ CZC

TORONTO BERKELEY

METHODS

CLASSICAL (SIM ANNEALING)

E. K.-H. Lee, Y. B. Kim,
PRB 91, 064407 (2015)

SOFT-SPIN (MIX BY HAND)

I KIMCHI, R COLDEA, A VISHWANATH
PRB 91, 245134 (2015)

Comparison Study

		CLASSICAL (SIM ANN)	SOFT-SPIN	
			No Mix	Mix
JKΓ TORONTO	β	same as exp		
	γ	Non-coplanar (a, wrong, c)		
CZC BERKELEY	β		co-planar (a, zero, c)	same as exp
	γ		co-planar (a, zero, c)	same as exp

EKH LEE, J RAU, YB KIM
arXiv:150606746 (2015)

Comparison Study

		CLASSICAL (SIM ANN)	SOFT-SPIN	
			No Mix	Mix
JKΓ TORONTO	β	same as exp		
	γ	Non-coplanar (a, wrong, c)		
CZC BERKELEY	β	Commensurate	co-planar (a, zero, c)	same as exp
	γ	Commensurate	co-planar (a, zero, c)	same as exp

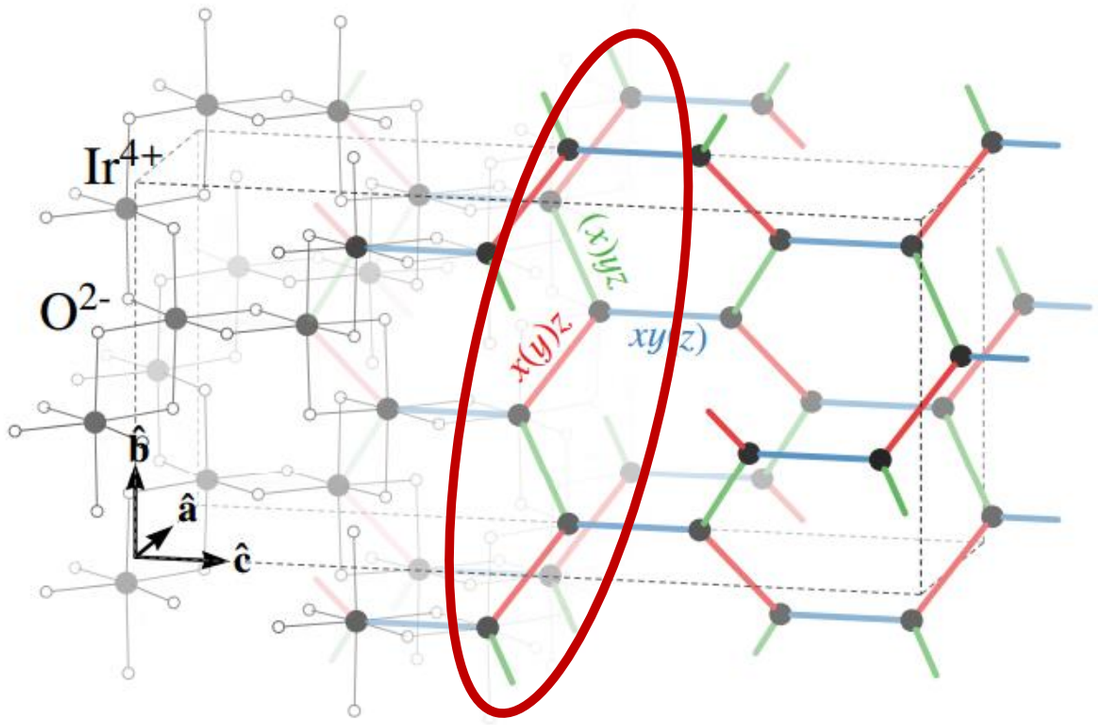
EKH LEE, J RAU, YB KIM
arXiv:150606746 (2015)

Comparison Study

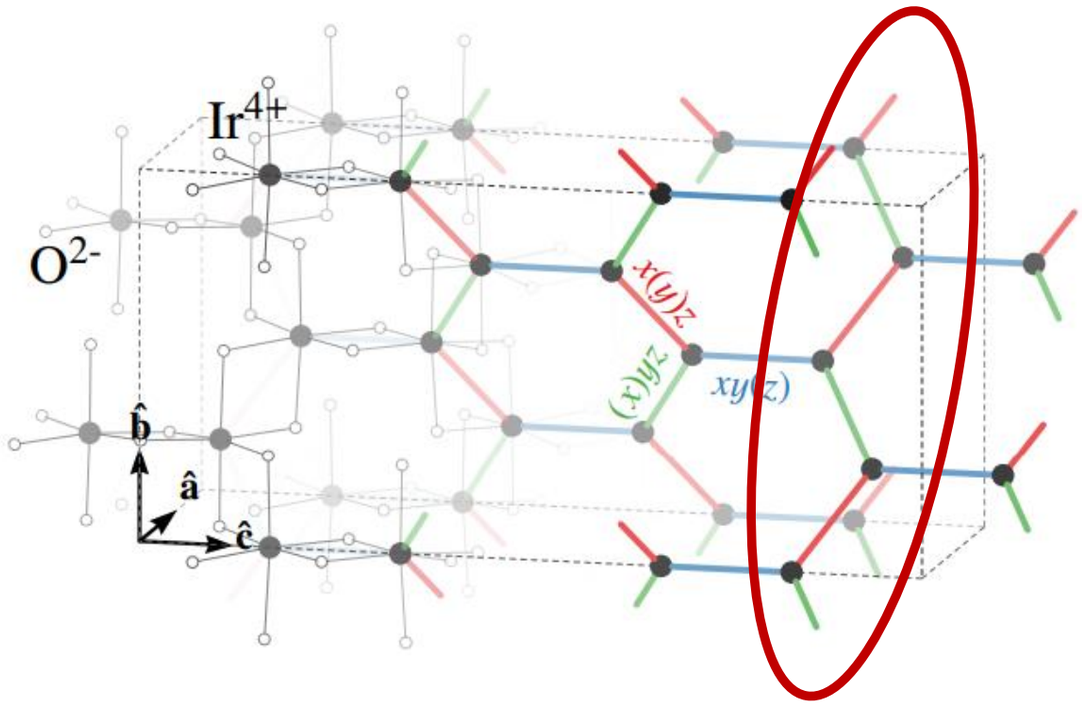
		CLASSICAL (SIM ANN)	SOFT-SPIN	
			No Mix	Mix
JKΓ TORONTO	β	same as exp	same as exp	No need
	γ	Non-coplanar (a, wrong, c)	Non-coplanar (a, wrong, c)	same as exp
CZC BERKELEY	β	Commensurate	co-planar (a, zero, c)	same as exp
	γ	Commensurate	co-planar (a, zero, c)	same as exp

EKH LEE, J RAU, YB KIM
arXiv:150606746 (2015)

Decoupled Chain Limit



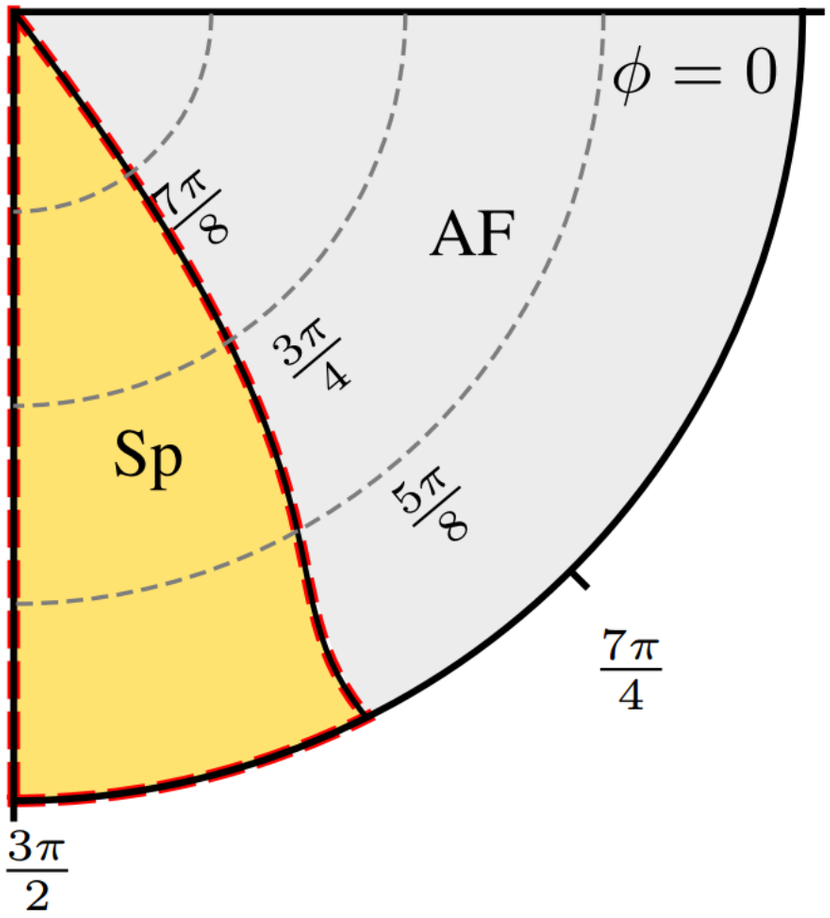
HYPERHONEYCOMB



STRIPYHONEYCOMB

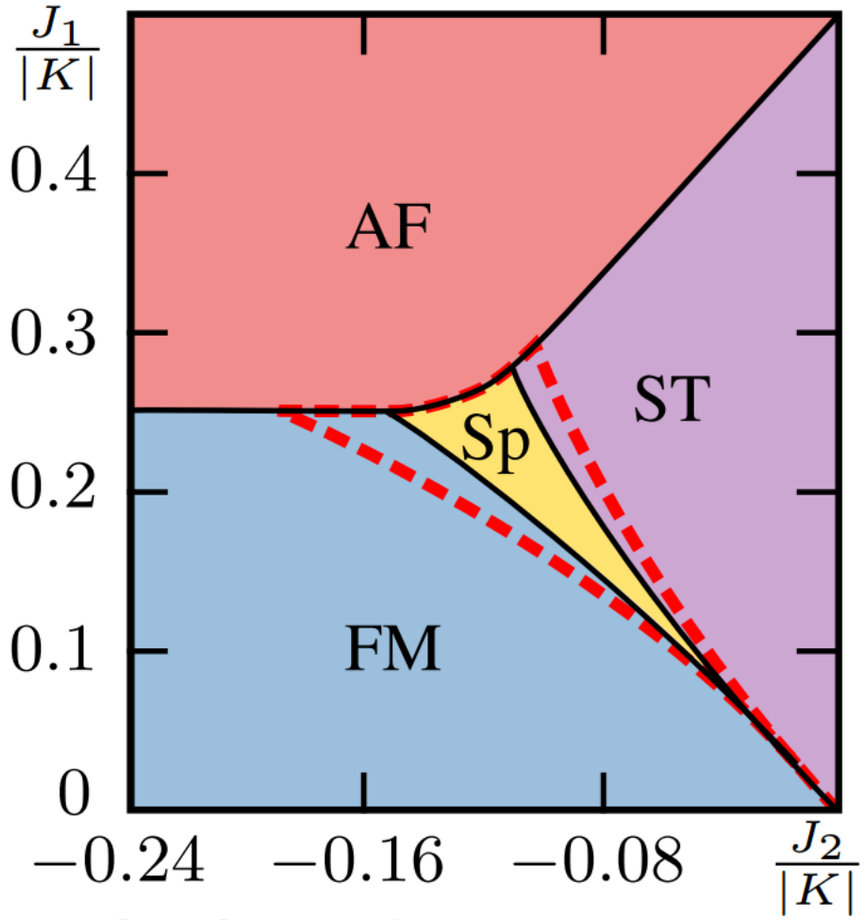
EKH LEE, J RAU, YB KIM
arXiv:150606746 (2015)

Decoupled Chain Limit - Classical



JKΓ TORONTO

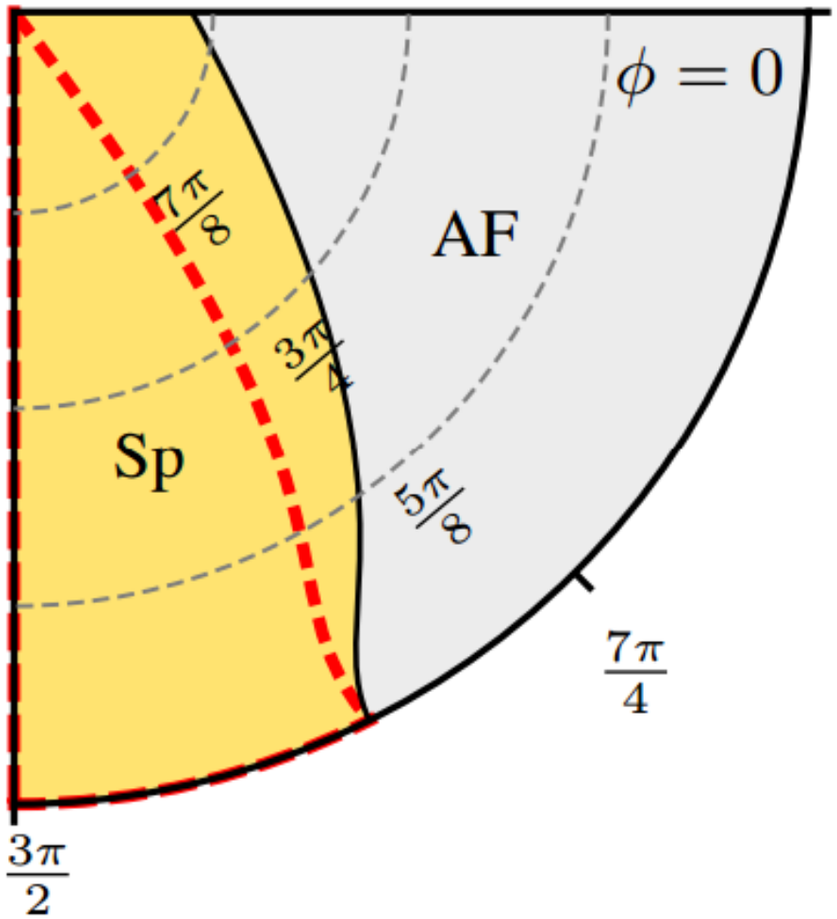
EKH LEE, J RAU, YB KIM
arXiv:150606746 (2015)



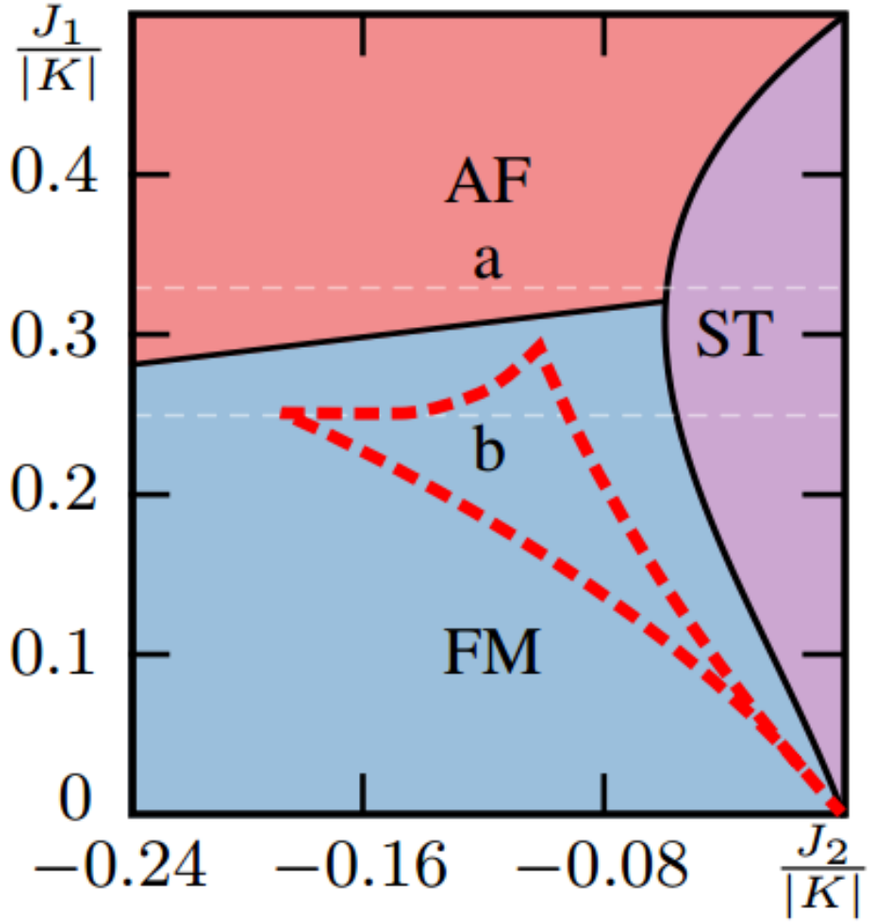
CZC+J2 BERKELEY

I KIMCHI, R COLDEA, A VISHWANATH
PRB 91, 245134 (2015)

Decoupled Chain Limit - DMRG



JKΓ TORONTO



CZC+J2 BERKELEY

EKH LEE, J RAU, YB KIM
arXiv:150606746 (2015)

Decoupled Chain Limit - DMRG

Intra-chain Γ interaction is important for the stabilization of incommensurate spiral order in the 1D quantum model

Inter-chain Γ interaction may be important for CZC (coupled zig-zag chain) model in 3D ? will need 3D quantum model

EKH LEE, J RAU, YB KIM
arXiv:150606746 (2015)

Why do we care (no spin liquid) ?

This is a benchmark for Kitaev interaction

Engineering Kitaev limit (relative strength of Ir-Ir and Ir-O-Ir exchanges)

The Kitaev interaction may be dominant in the 3D materials, irrespective of details
Pressure exp (Takagi): gapless spin liquid ?

Finite temperature signatures

Need understanding of Quantum Model